QCD, Capability Computing, and Sustainable Stewardship

J.W. Negele

Advanced Simulation & Computing

Principal Investigator's Meeting

Las Vegas, February 21, 2007

Outline

What have we done for you lately?
What can we do in the future?

- Fundamental physics:
  Understanding strong interactions from first principles
- Capability hardware:
  From the QCDSP to the BG/L, BG/P and BG/Q
- Optimized platform-independent software

Fundamental physics

- How do nucleons and their interactions arise from QCD?
- Lagrangian constrained by Lorentz invariance, gauge invariance and renormalizability:

$$\mathcal{L} = \bar{\psi}(i\gamma^{\mu} D_{\mu} - m)\psi - \frac{1}{4}F^2_{\mu\nu}$$

$$D_{\mu} = \partial_{\mu} - igA_{\mu} \qquad F_{\mu\nu} = \frac{i}{g}[D_{\mu}, D_{\nu}]$$

- Deceptively simple Lagrangian produces amazingly rich and complex structure of strongly interacting matter in our universe

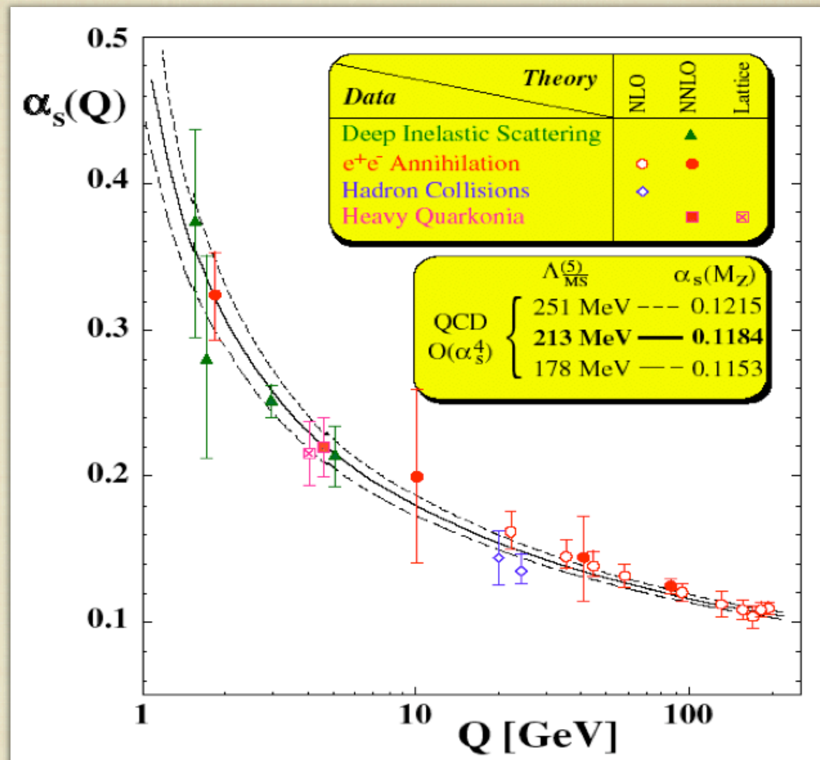
QCD and Asymptotic Freedom

David J. Gross
Kavli Institute for Theoretical Physics
University of California, Santa Barbara, USA

H. David Politzer
California Institute of Technology (Caltech), Pasadena, USA

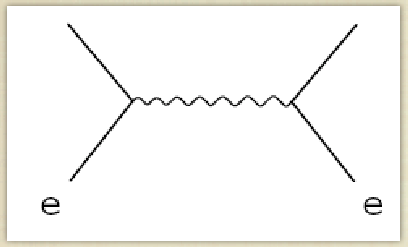
Frank Wilczek
Massachusetts Institute of Technology (MIT), Cambridge, USA

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Physics for 2004 "for the discovery of asymptotic freedom in the theory of the strong interaction" jointly to David J. Gross, H. David Politzer and Frank Wilczek

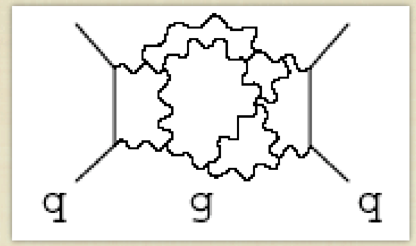


Nonperturbative QCD

QED



QCD



- Fundamental differences relative to QED
  - Self-interacting: highly nonlinear
  - Interaction increases at large distance: Confinement
  - Interaction decreases at small distance: Asymptotic Freedom
  - Strong coupling: $\alpha_s \gg \alpha_{em}$
  - Topological excitations
- Solution of QCD
  - Present analytical techniques inadequate
  - Numerical evaluation of path integral on space-time lattice

Basic Ideas in Lattice QCD

Basic Ideas in Lattice QCD

Evolution in Euclidean time

$$|\psi\rangle \equiv \sum_n e^{-\beta E_n} C_n |\psi_n\rangle \to C_0 e^{-\beta E_0} |\psi_0\rangle$$

Basic Ideas in Lattice QCD

Evolution in Euclidean time

$$|\psi\rangle \equiv \sum_n e^{-\beta E_n} C_n |\psi_n\rangle \rightarrow C_0 e^{-\beta E_0} |\psi_0\rangle$$

Lattice Regularization

$$\phi(x) \rightarrow \phi(x_n), \quad x_n = na$$

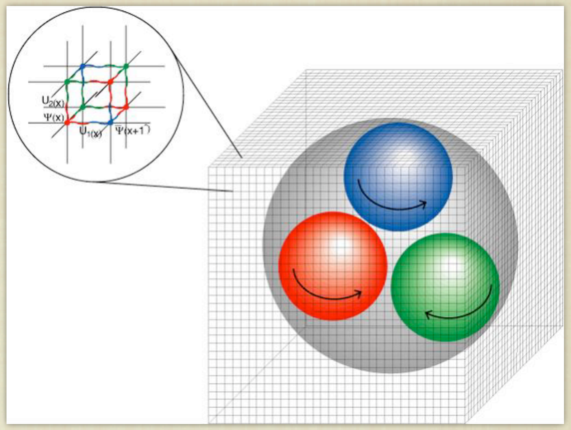
Basic Ideas in Lattice QCD

Evolution in Euclidean time

$$|\psi\rangle \equiv \sum_n e^{-\beta E_n} C_n |\psi_n\rangle \to C_0 e^{-\beta E_0} |\psi_0\rangle$$

Lattice Regularization

$$\phi(x) \to \phi(x_n), \quad x_n = na$$



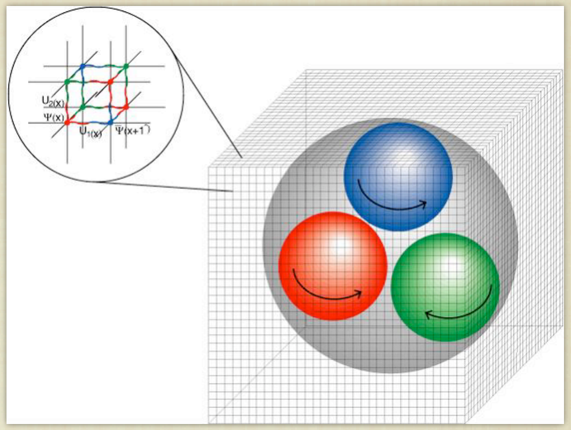
Basic Ideas in Lattice QCD

Evolution in Euclidean time

$$|\psi\rangle \equiv \sum_n e^{-\beta E_n} C_n |\psi_n\rangle \rightarrow C_0 e^{-\beta E_0} |\psi_0\rangle$$

Lattice Regularization

$$\phi(x) \rightarrow \phi(x_n), \quad x_n = na$$



Path Integral

$$e^{-\beta \hat{H}} \rightarrow \int D[x(\tau)] e^{-\int_0^\beta d\tau S[x(\tau)]}$$

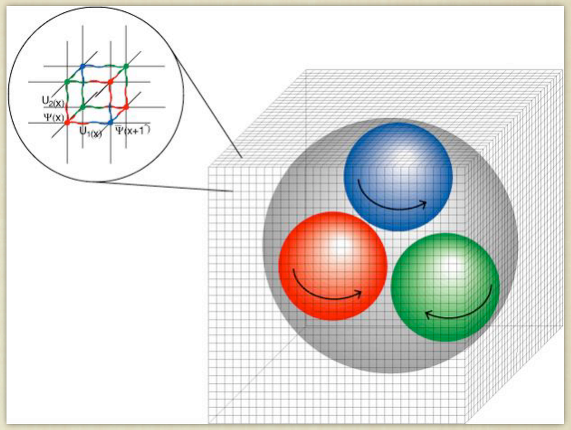
Basic Ideas in Lattice QCD

Evolution in Euclidean time

$$|\psi\rangle \equiv \sum_n e^{-\beta E_n} C_n |\psi_n\rangle \to C_0 e^{-\beta E_0} |\psi_0\rangle$$

Lattice Regularization

$$\phi(x) \to \phi(x_n), \quad x_n = na$$



Path Integral

$$e^{-\beta \hat{H}} \to \int D[x(\tau)] e^{-\int_0^\beta d\tau S[x(\tau)]}$$

Stochastic Solution

$$\int dx f(x) P(x) = \frac{1}{N} \sum_{x_i \in P} f(x_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

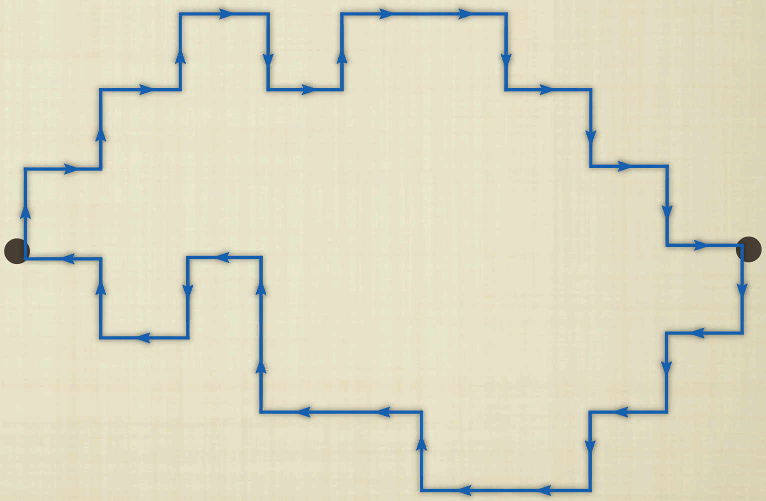
•

•

Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

- $M^{-1} = (1+\kappa U)^{-1}$ connects Ψ's with line of U's
  Sum over valence quark paths

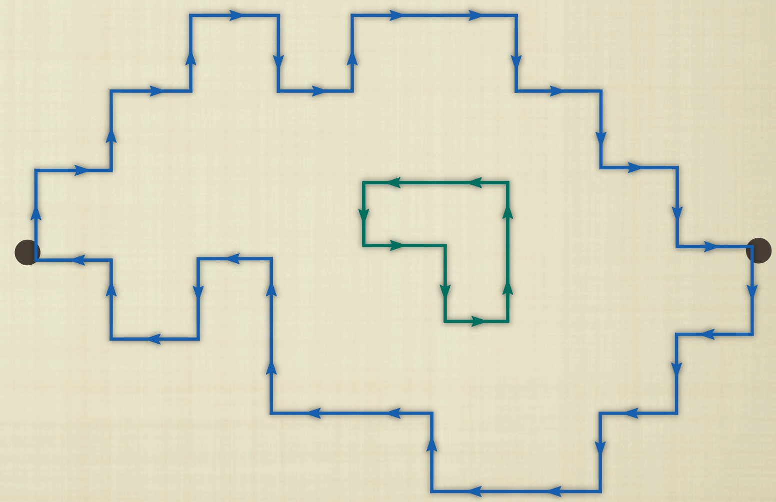


Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

- $M^{-1} = (1+ \kappa U)^{-1}$ connects Ψ's with line of U's
  Sum over valence quark paths

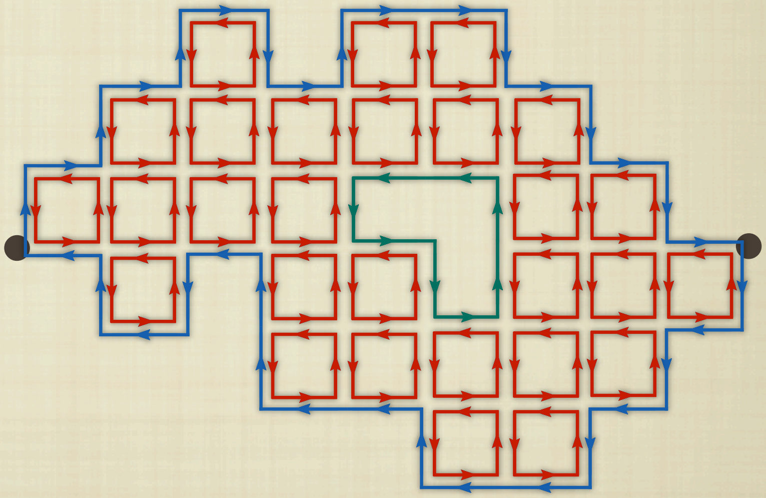
- det M generates closed loops of U's
  Sum over sea quark excitations



Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

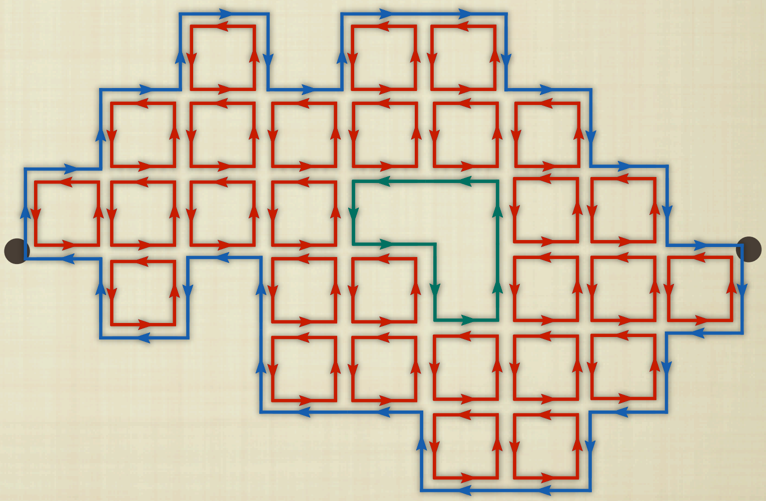
- $M^{-1} = (1 + \kappa U)^{-1}$ connects Ψ's with line of U's
  Sum over valence quark paths
- det M generates closed loops of U's
  Sum over sea quark excitations
- S(U) tiles with plaquettes
  → Sum over all gluons



Lattice QCD - summing over paths

$$\langle T\, e^{-\beta H} \psi\psi\psi \cdots \bar{\psi}\bar{\psi}\bar{\psi} \rangle = \prod_n \int dU_n \frac{1}{Z} \det M(U) e^{-S(U)} \sum M^{-1}(U) M^{-1}(U) \cdots M^{-1}(U)$$

- $M^{-1} = (1 + \kappa\, U)^{-1}$ connects Ψ's with line of U's
  Sum over valence quark paths
- det M generates closed loops of U's
  Sum over sea quark excitations
- S(U) tiles with plaquettes
  → Sum over all gluons
- $32^3 \times 64$ lattices → 10^8 gluon variables



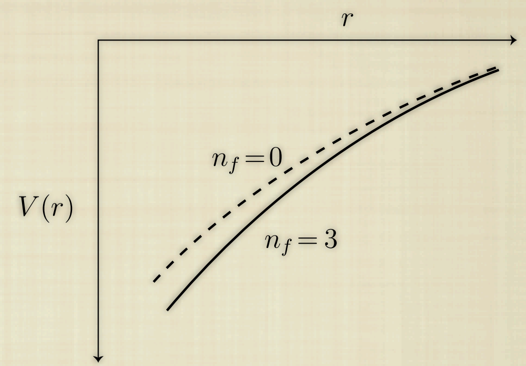
Computational Issues

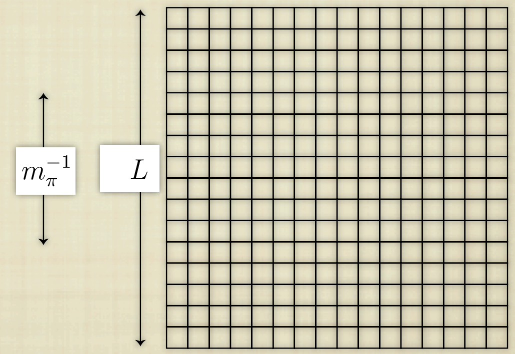
- Fermion determinant - Full QCD
- Small lattice spacing
- Small quark mass
- Large lattice volume

$$\frac{1}{m_\pi} \leq \frac{L}{4}$$

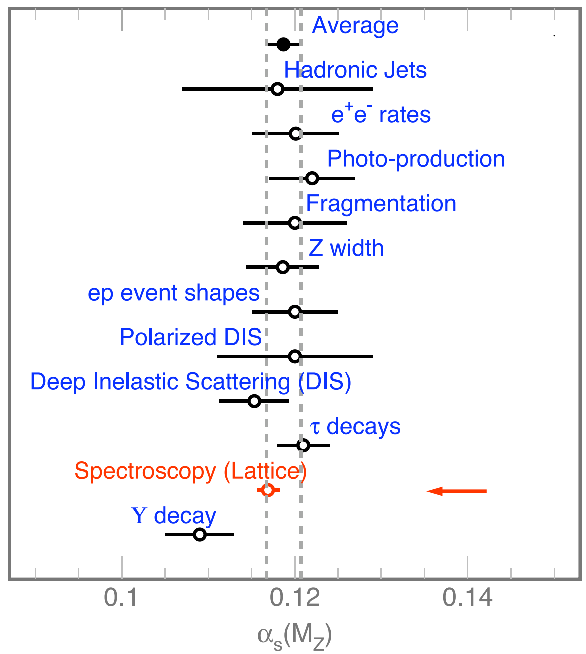
L(fm)	m_π (Mev)
1.6	500
4.0	200
5.7	140

- Cost ~ $(m_\pi)^{-7}$ - $(m_\pi)^{-9}$





Precision agreement in heavy quark systems

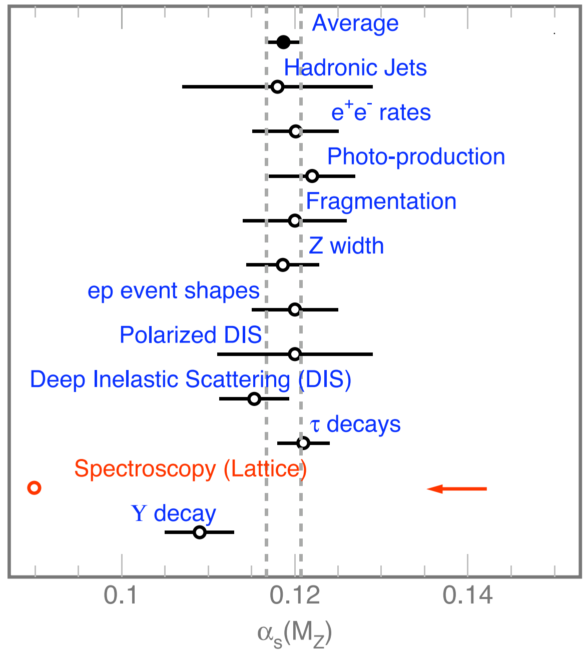


Mason et al, hep-lat/0503005v1 (2005); Particle Data Group (2004)

$\alpha_s(M_Z)$ from Particle Data Group

Precision agreement in heavy quark systems

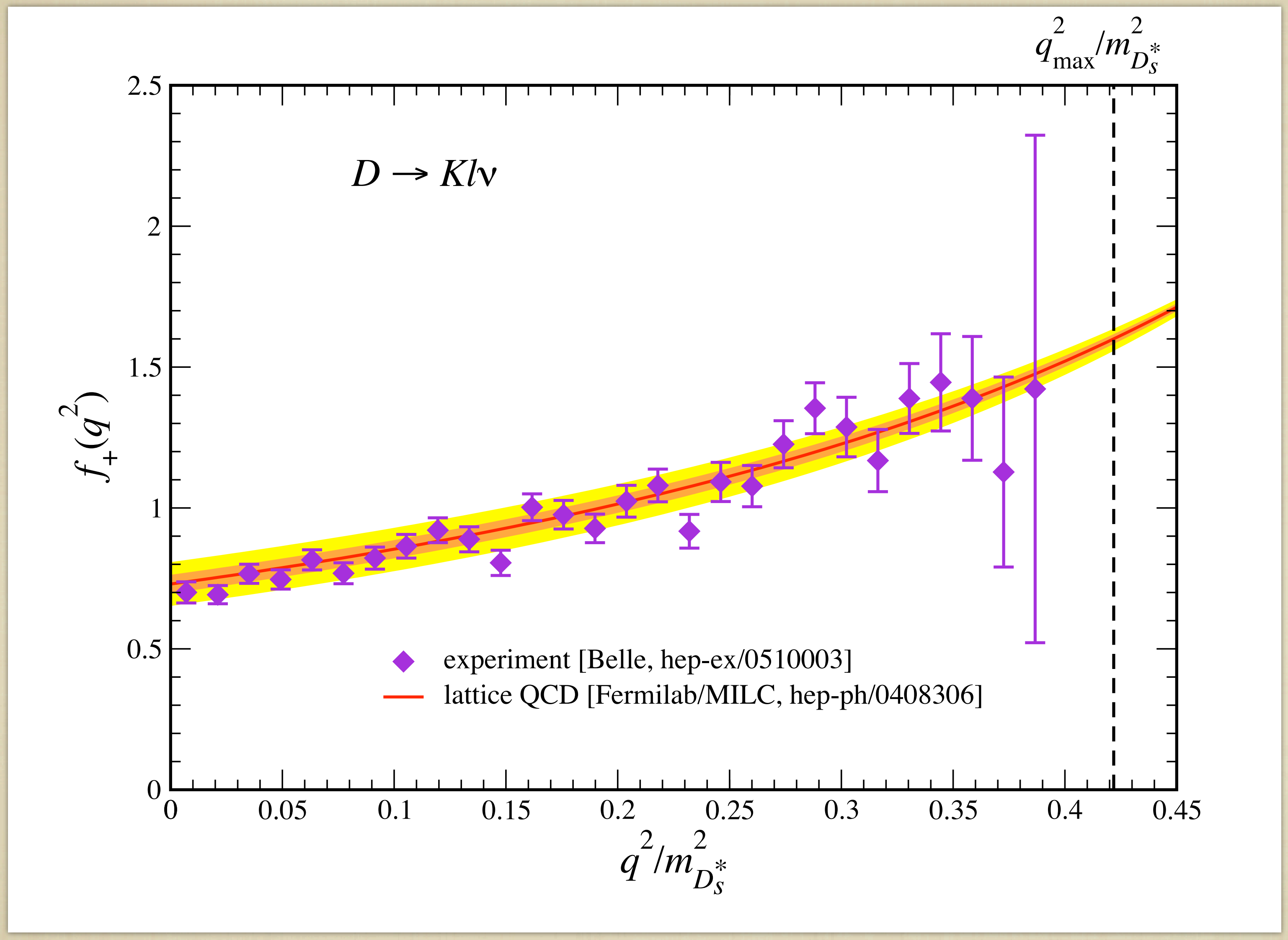
And without light-quark vacuum polarization:



Mason et al, hep-lat/0503005v1 (2005); Particle Data Group (2004)

$\alpha_s(M_Z)$ from Particle Data Group

Lattice QCD Predictions



Highlights of lattice results

- In 2006, lattice QCD, ~ 50 sustained Tflops-yrs devoted to lattice QCD
- Survey highlights in:
  - Hadron structure
  - QCD thermodynamics
  - Hadron interactions

Collaborators

MIT
- B. Bistrovic
- J. Bratt
- D. Dolgov
- O. Jahn
- A. Pochinsky
- D. Sigaev

JLab
- R. Edwards
- D. Richards

William & Mary, JLab
- K. Orginos

Arizona
- D. Renner

Yale
- G. Fleming

T. U. Munchen
- Ph. Haegler
- B. Musch

DESY Zeuthen
- W. Schroers

U Cyprus
- C. Alexandrou
- G. Koutsou
- Ph. Leontiou

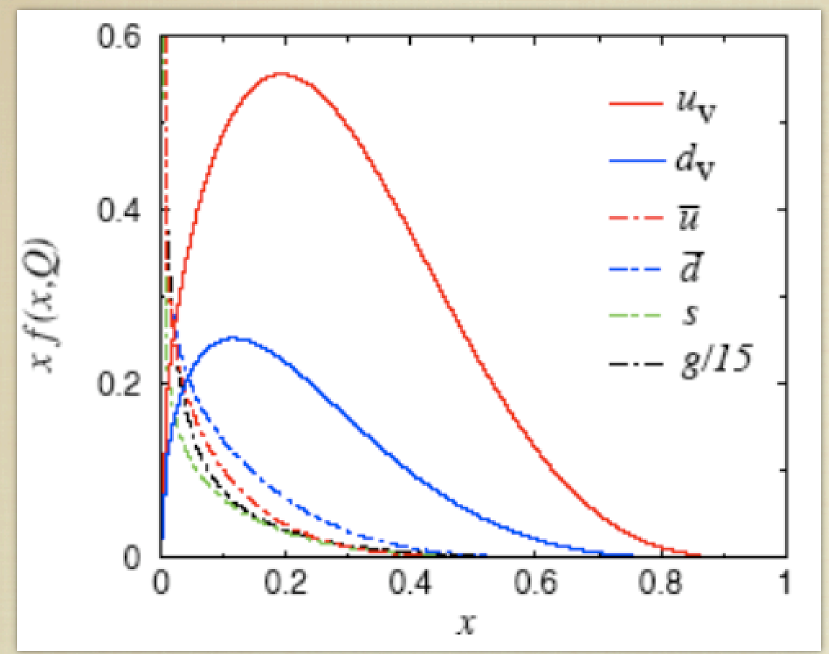
Athens
- A. Tsapalis

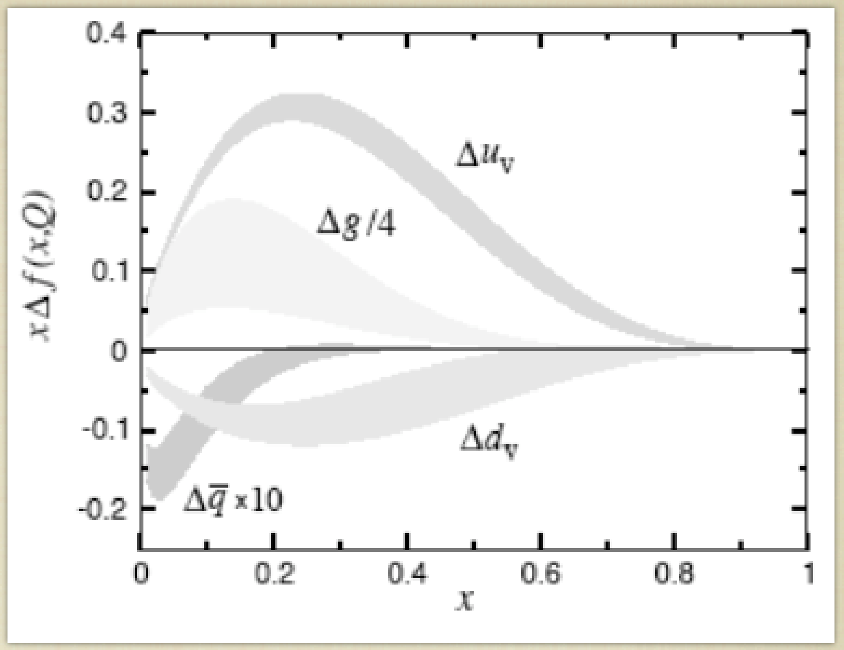
ETH, CERN
- Ph. de Forcrand

Julich
- Th. Lippert

Wuppertal
- K. Schilling

Moments of parton distributions





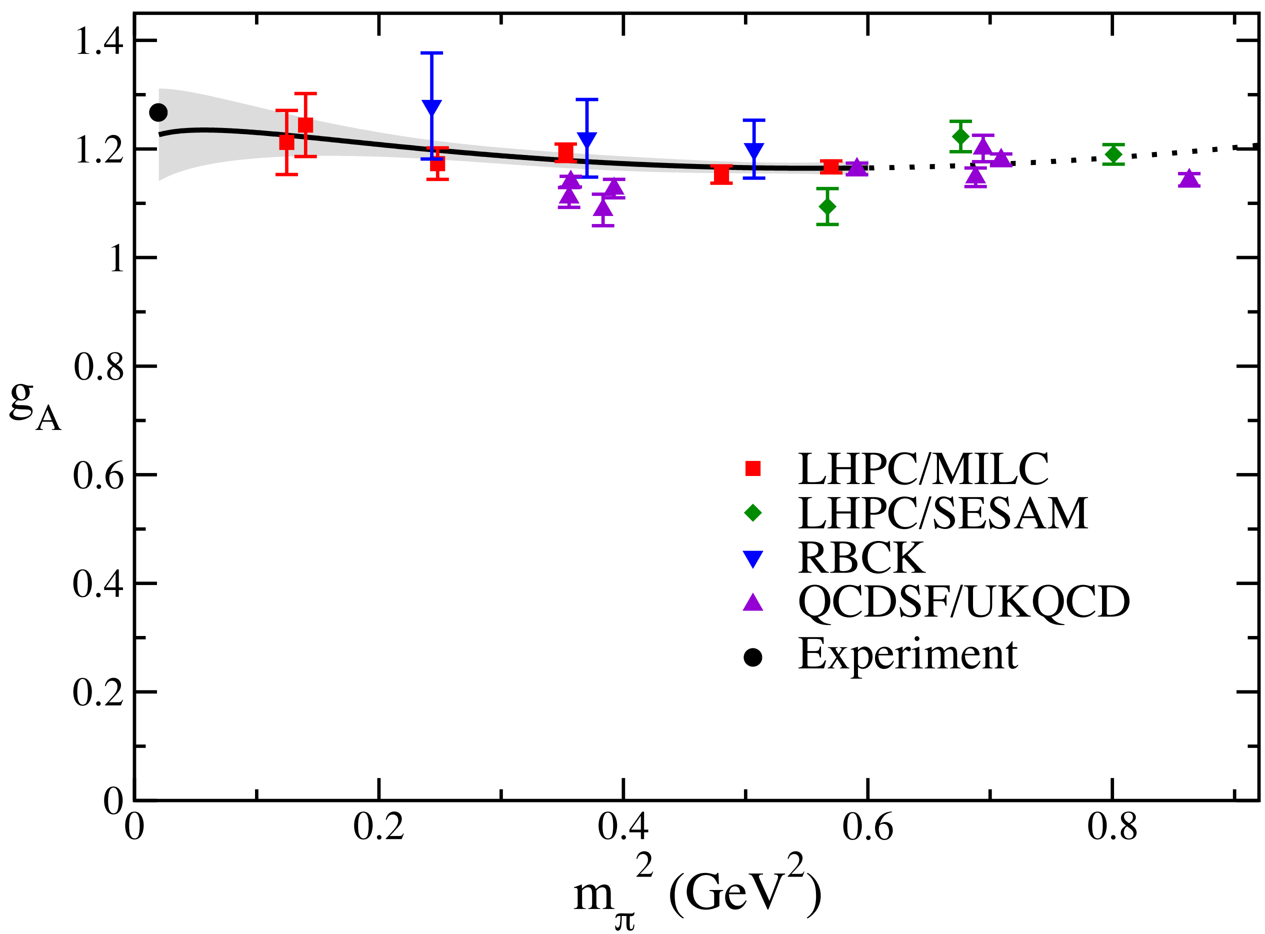
$$\langle p|\bar{\psi}\gamma_\mu D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \quad \langle x^n\rangle_q \quad = \int_0^1 dx x^n[q(x)+(-1)^{(n+1)}\bar{q}(x)]$$

$$\langle p|\bar{\psi}\gamma_5\gamma_\mu D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \quad \langle x^n\rangle_{\Delta q} \quad = \int_0^1 dx x^n[\Delta q(x)+(-1)^{(n)}\Delta\bar{q}(x)]$$

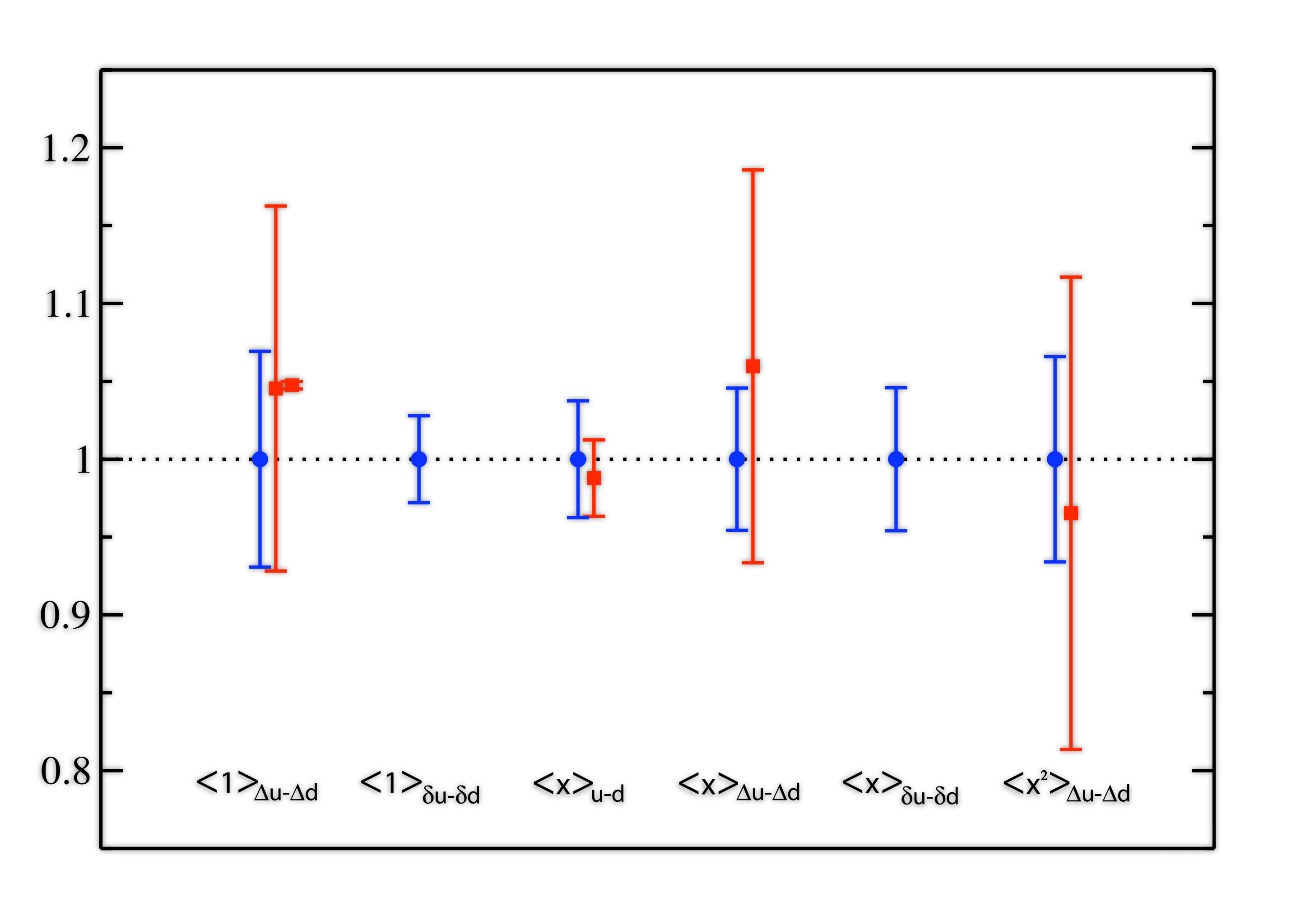
$$\langle p|\bar{\psi}\gamma_5\sigma_{\mu\nu} D_{\mu_1}\cdots D_{\mu_n}\psi|p\rangle \rightarrow \quad \langle x^n\rangle_{\delta q} \quad = \int_0^1 dx x^n[\delta q(x)+(-1)^{(n+1)}\delta\bar{q}(x)]$$

where $\quad q = q_\uparrow + q_\downarrow, \quad \Delta q = q_\uparrow - q_\downarrow, \quad \delta q = q_\top + q_\perp,$

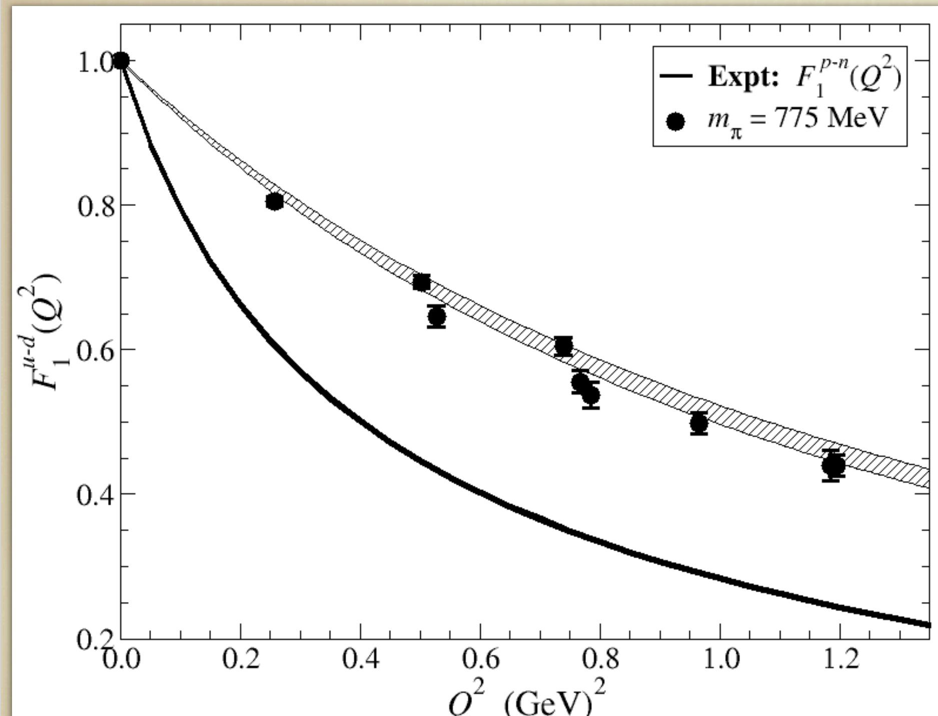
Nucleon axial charge g_A $\langle 1 \rangle_{\Delta q}^{u-d}$

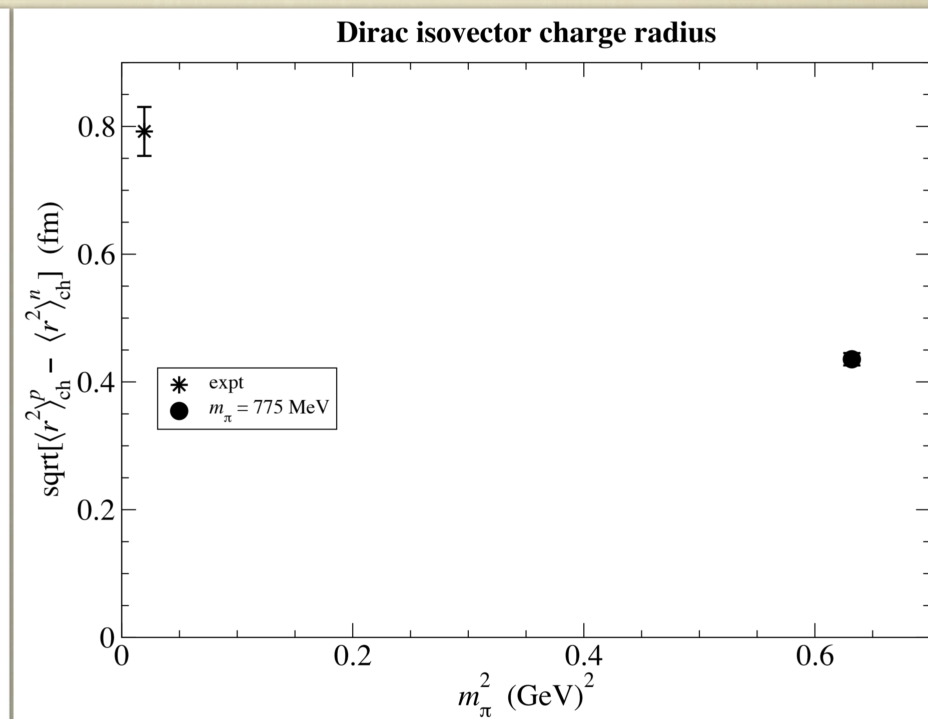


Chiral Extrapolation of Moments

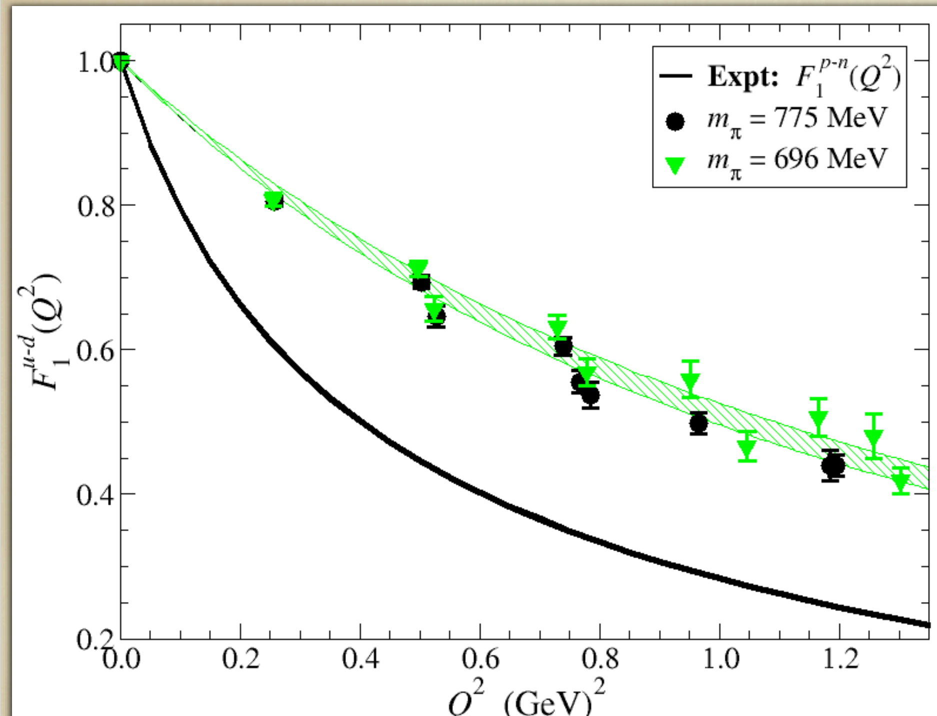


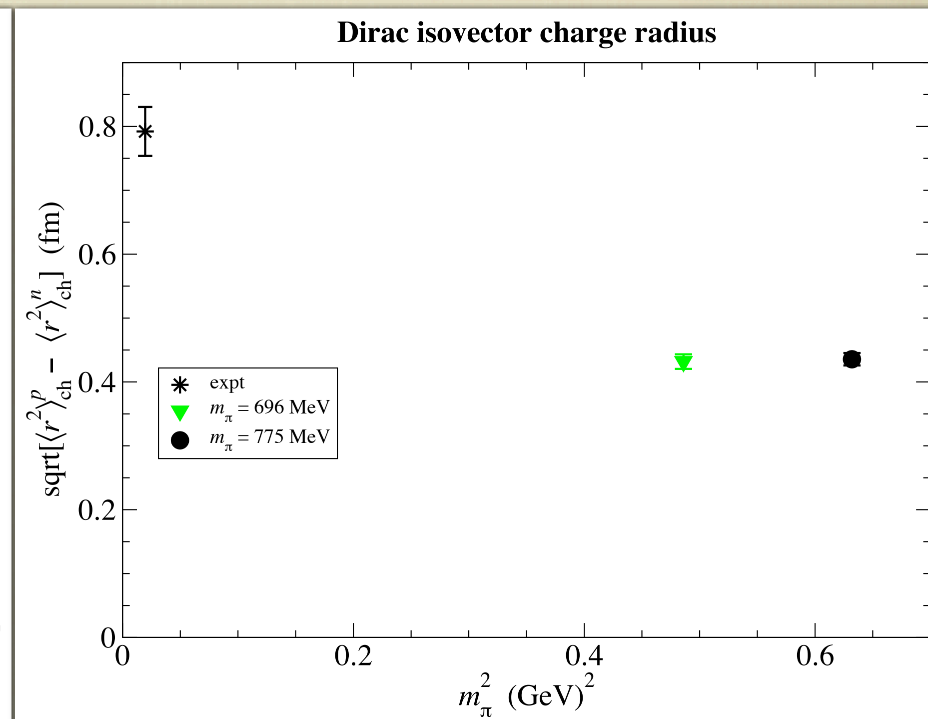
F_1 Isovector Form Factor



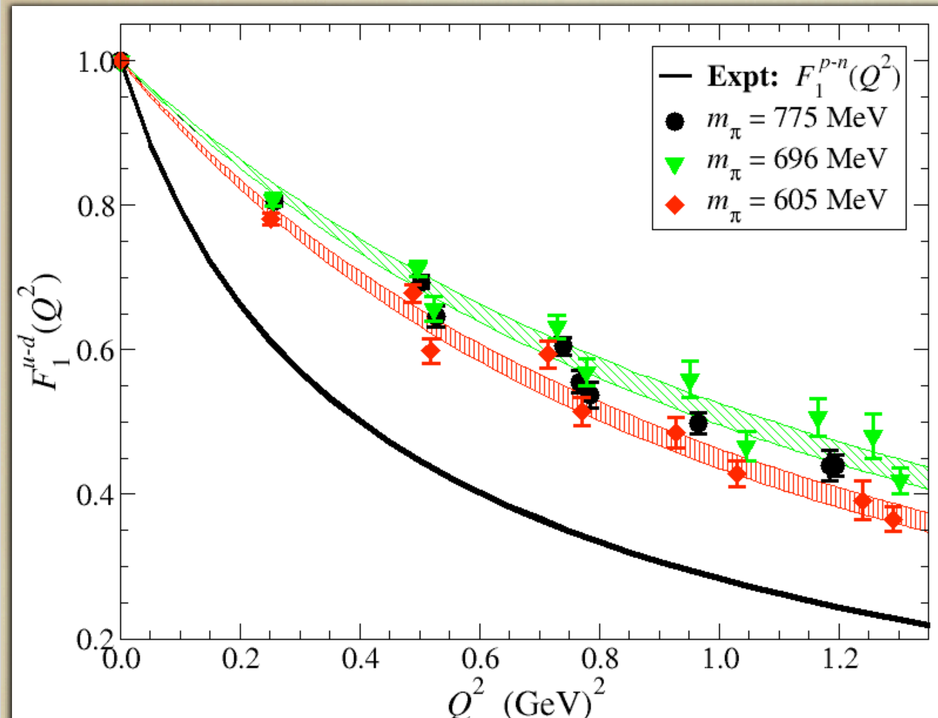


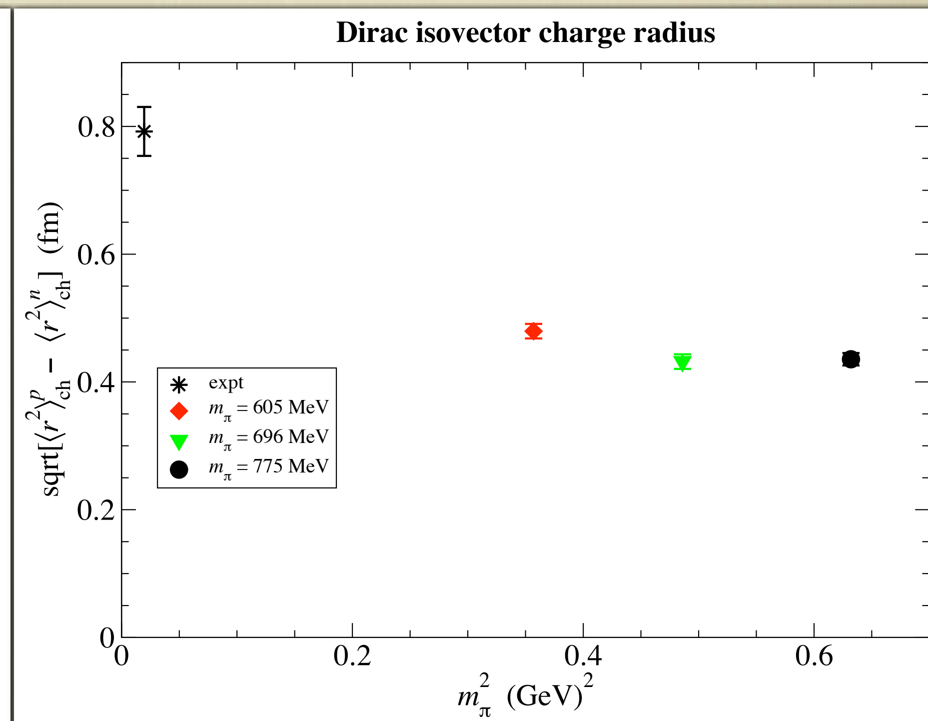
F_1 Isovector Form Factor



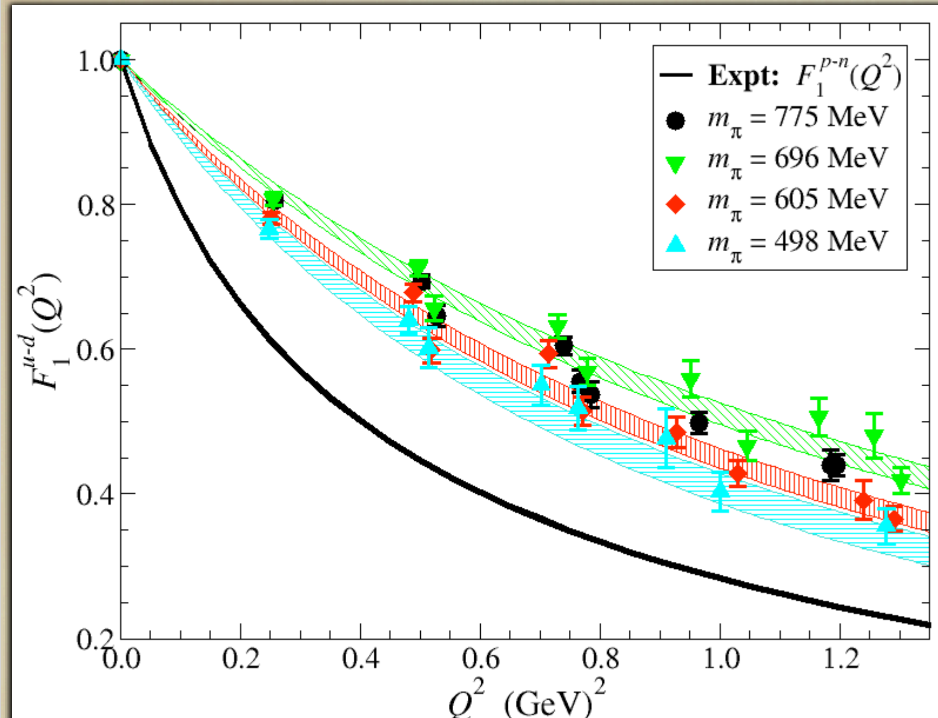


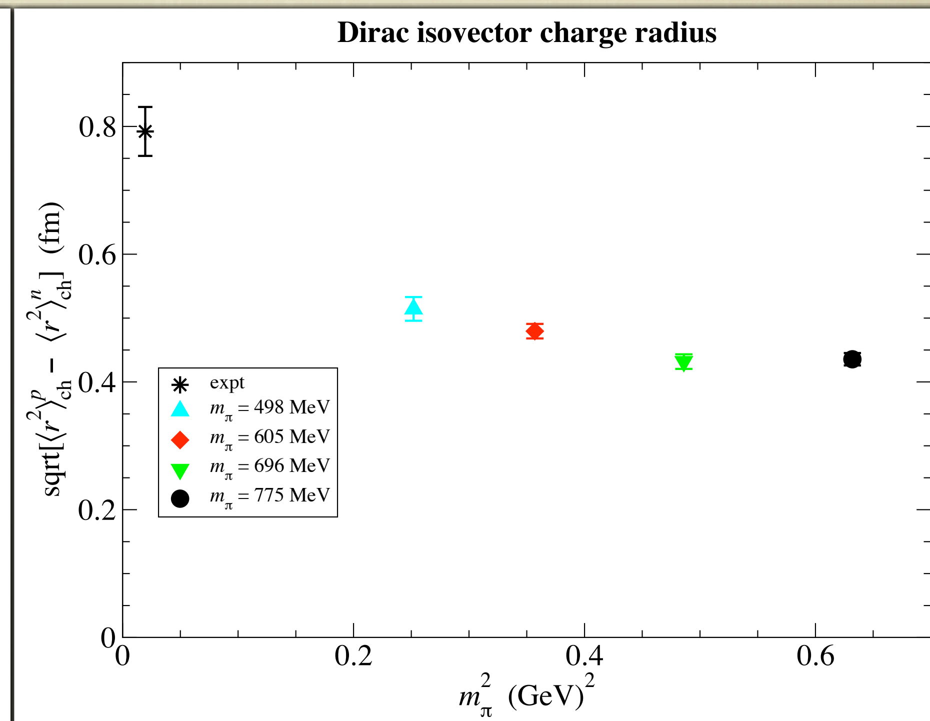
F_1 Isovector Form Factor



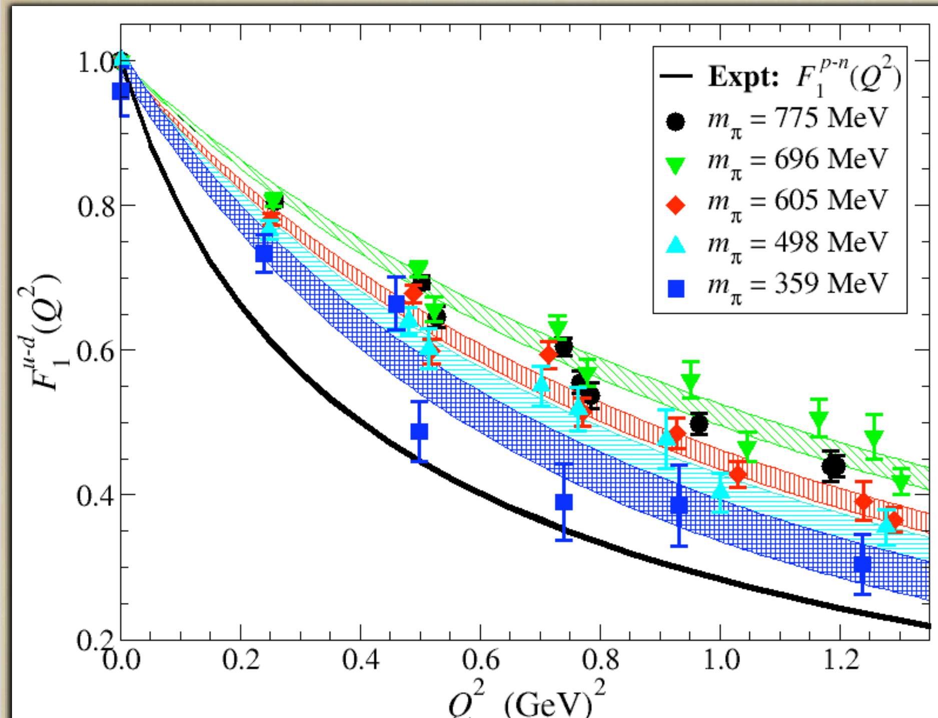


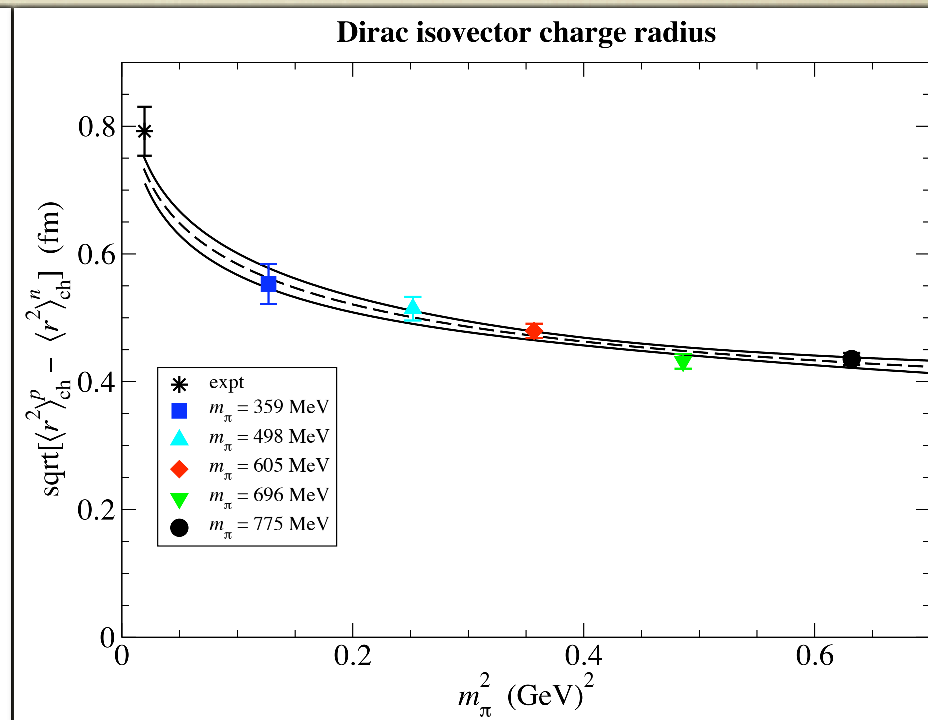
F_1 Isovector Form Factor





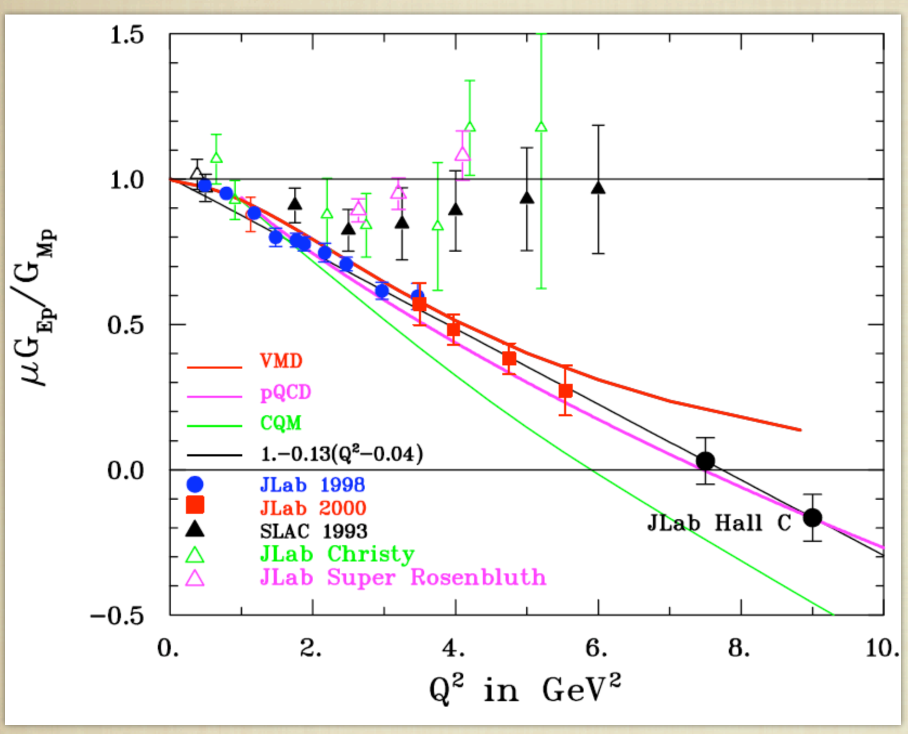
F_1 Isovector Form Factor

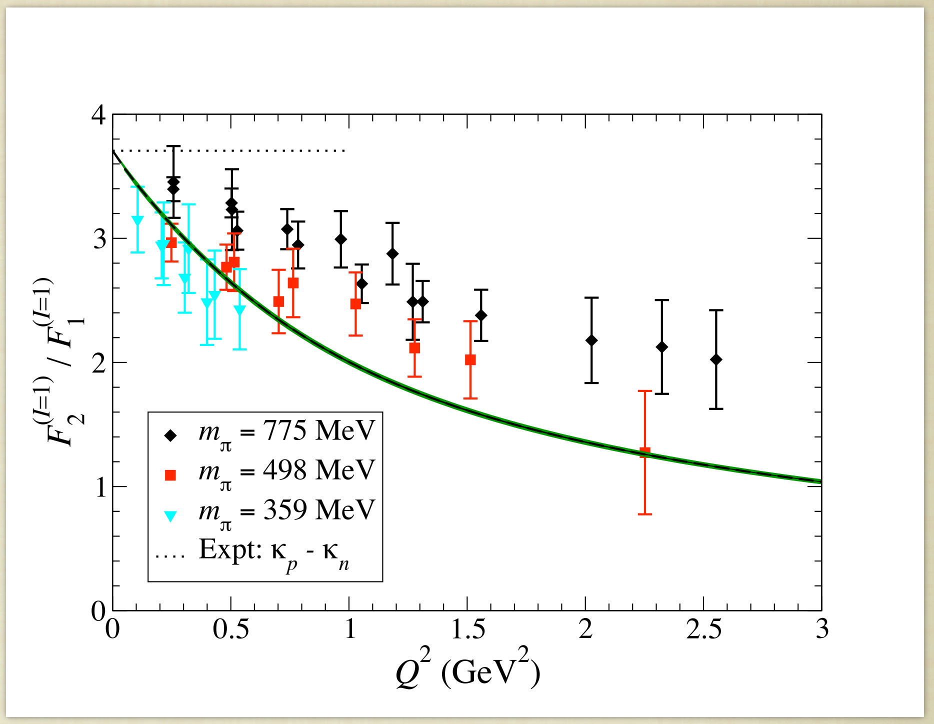




$$\langle r^2\rangle^{u-d} = a_0 - \frac{(1+5g_A^2)}{(4\pi f_\pi)^2}\log\left(\frac{m_\pi^2}{m_\pi^2+\Lambda^2}\right)$$

Form factor ratio: F_2 / F_1

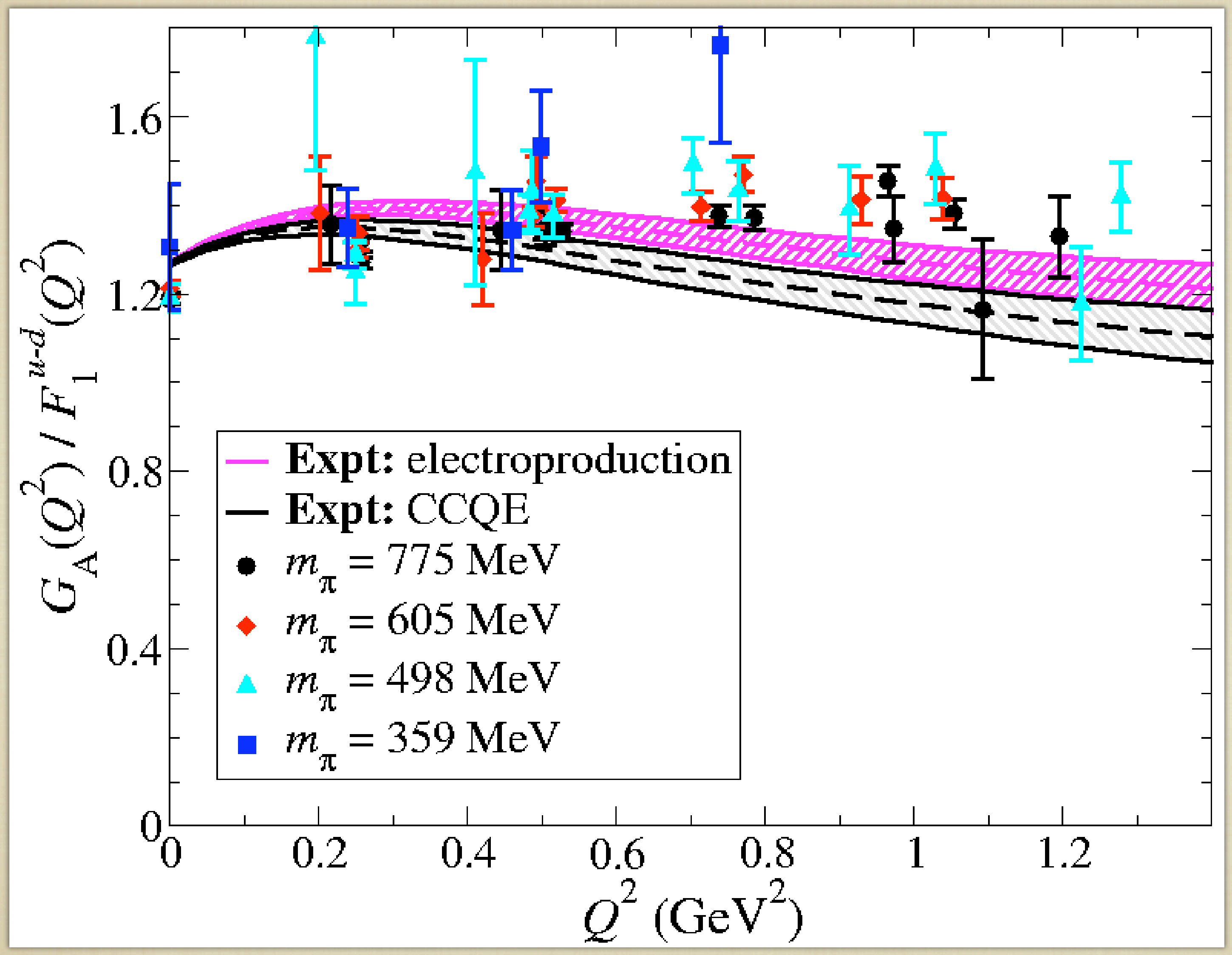




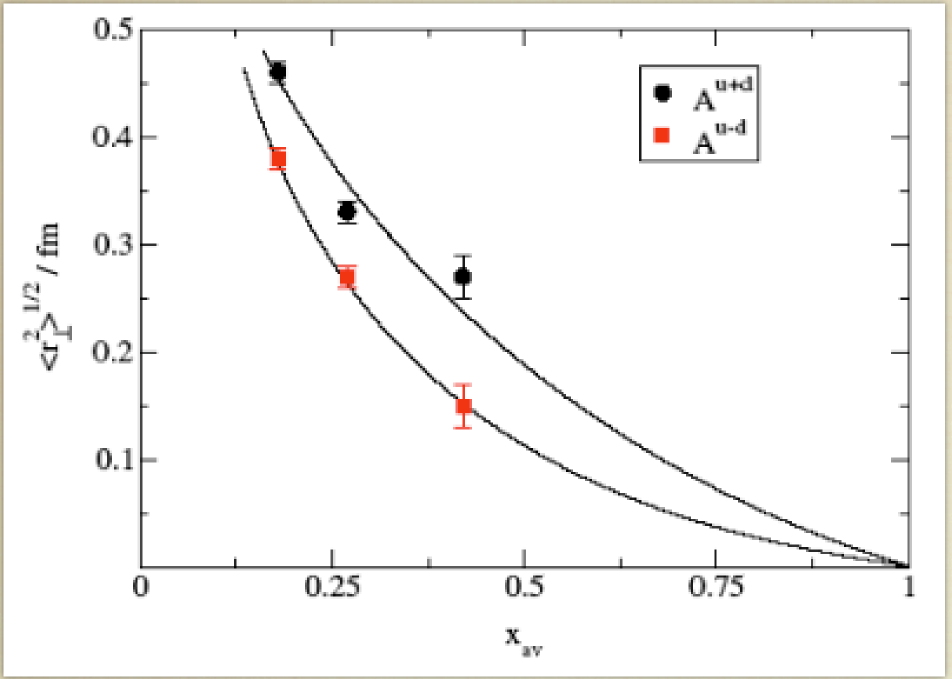
Polarization transfer at JLab

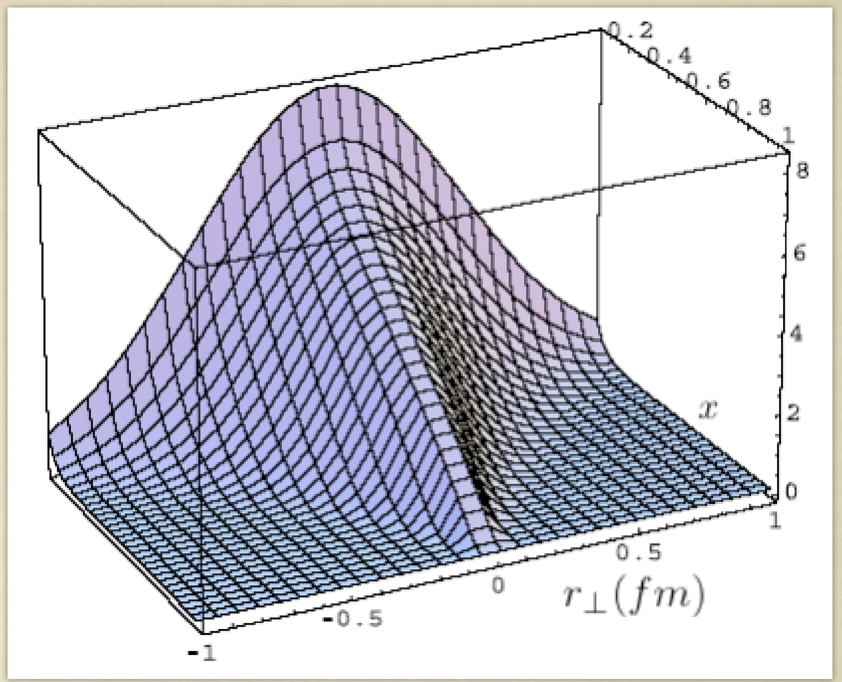
Lattice results

Form factor ratio: G_A/F_1



Transverse size of light-cone wave function

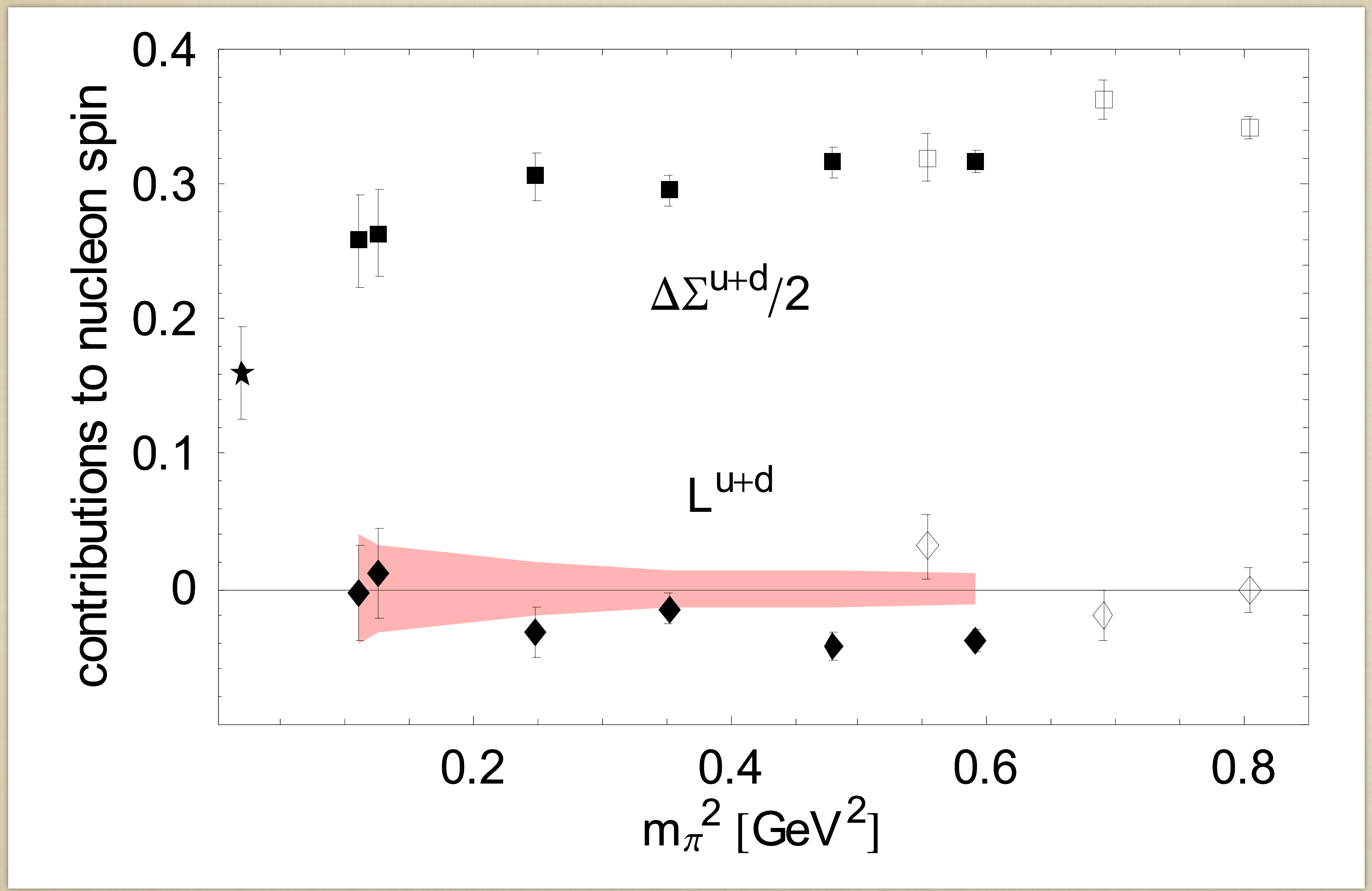




$$x_{\rm av}^n = \frac{\int d^2 r_\perp \int dx\, x \cdot x^{n-1} q(x, \vec{r}_\perp)}{\int d^2 r_\perp \int dx x^{n-1} q(x, \vec{r}_\perp)}$$

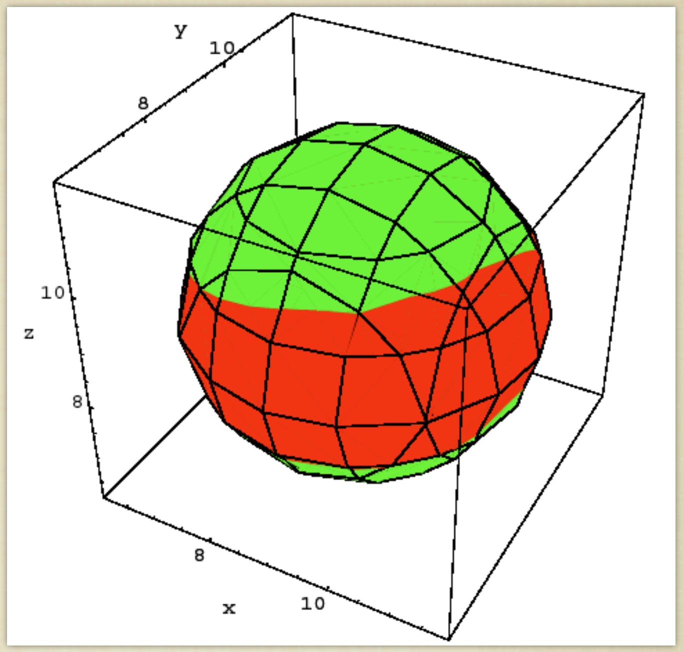
$q(x, \vec{r}_\perp)$ **model** (Burkardt hep-ph/0207047)

Nucleon spin decomposition



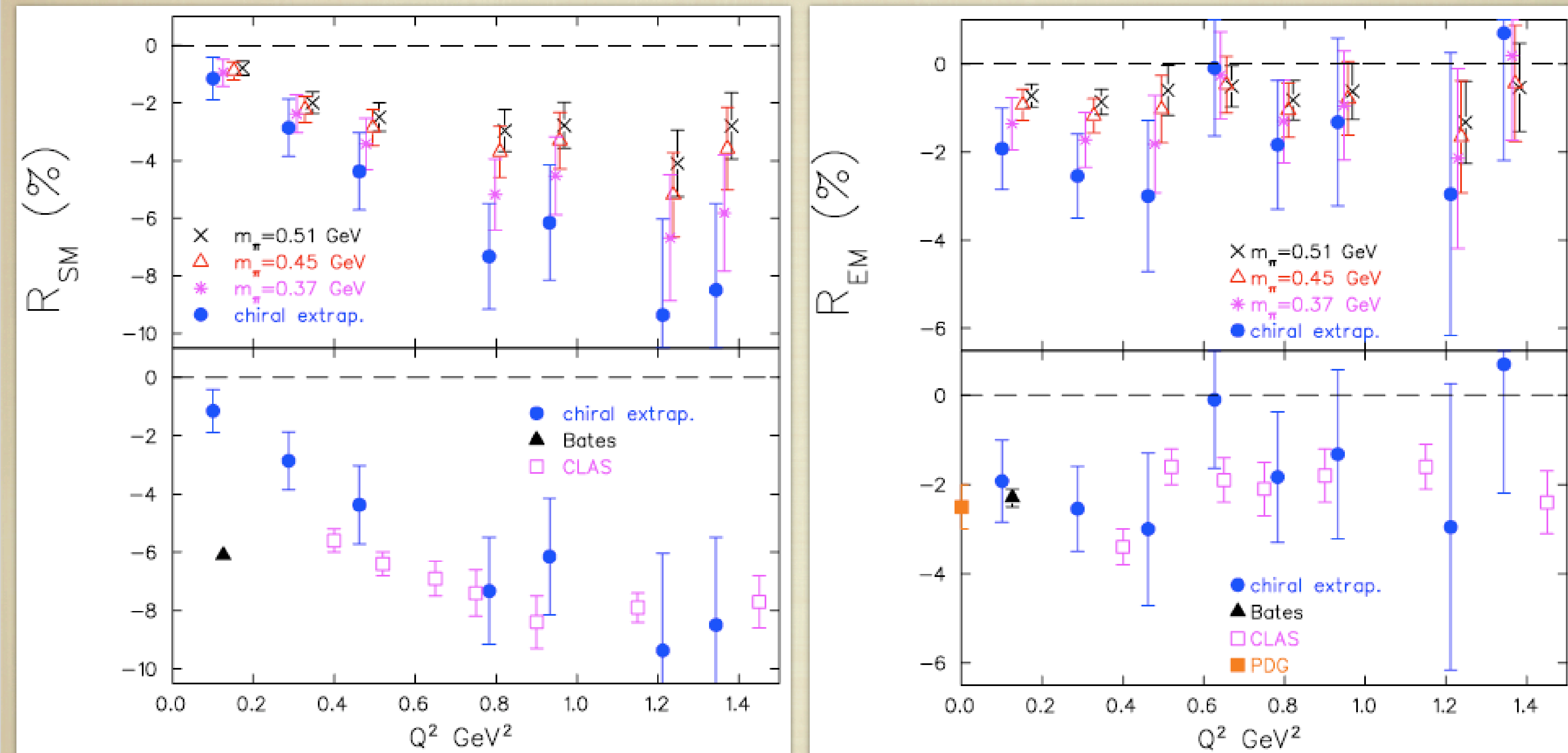
Baryon shapes

- Observe oblate deformation of spin 1/2 Δ directly on lattice from density-density correlation function (Alexandrou, nucl-th/0311007)



- Infer deformation experimentally from $N \rightarrow \Delta$ transition form factor
  - Dominant transition M1
  - C2 and E2 would vanish if nucleon and Δ spherical

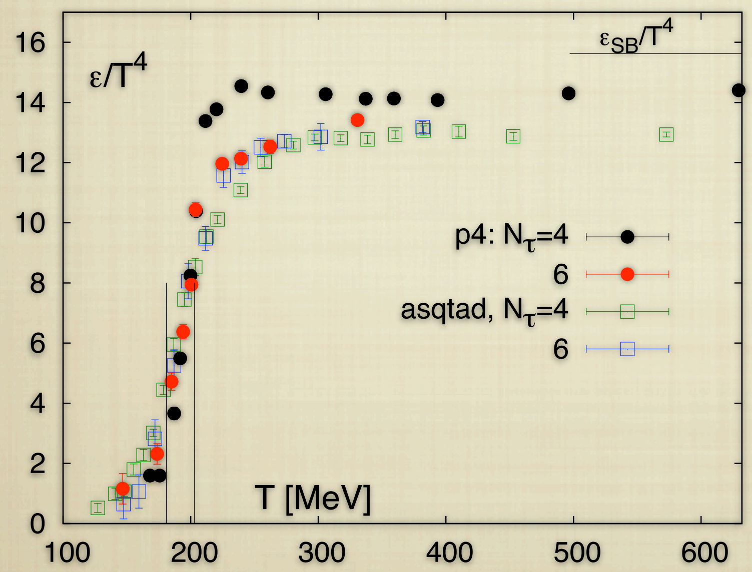
Electric and Coulomb transitions

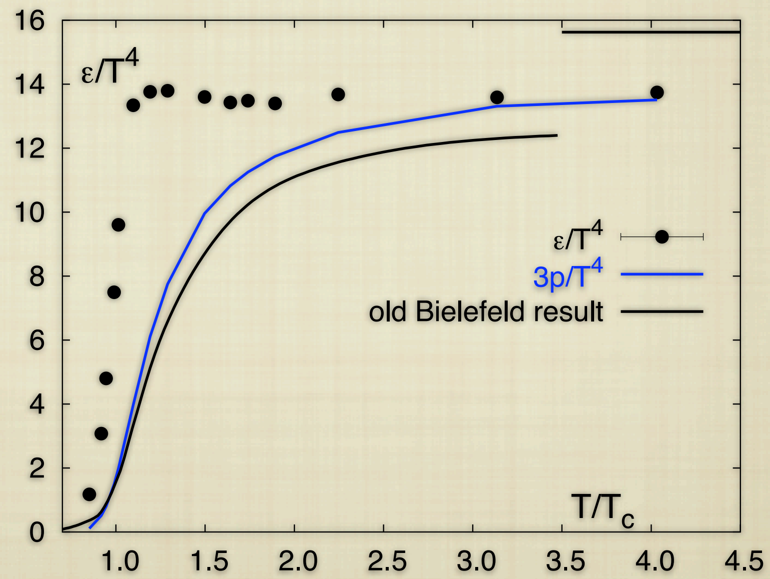


C2/M1 E2/M1

QCD Equation of State

- RHIC explores the phases of QCD
  - Quark-gluon plasma above T_C, confined below
  - Equation of state governs collision dynamics
- Errors due to coarse lattice and large quark mass
- Currently, Soltz, Karsch et al. calculating N = 8 (a ~ 0.13 fm) on LLNL BG



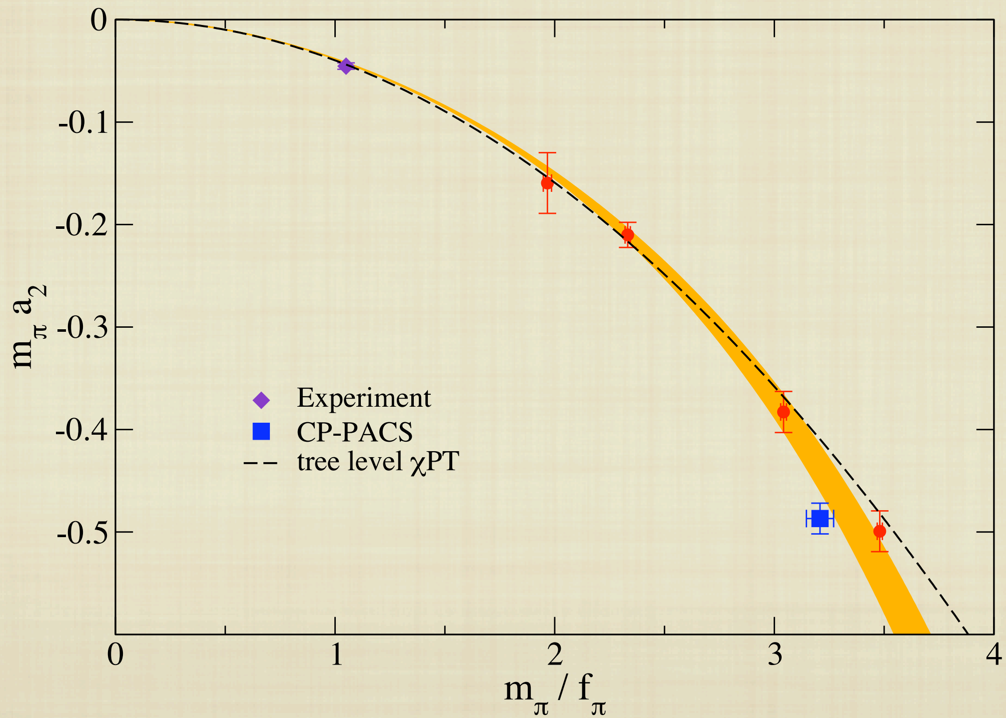


Results by Bielefeld, RBC, & MILC collaborations

I = 2 Pion scattering length

Calculate scattering length from energy variation with volume

Extrapolate with chiral perturbation theory

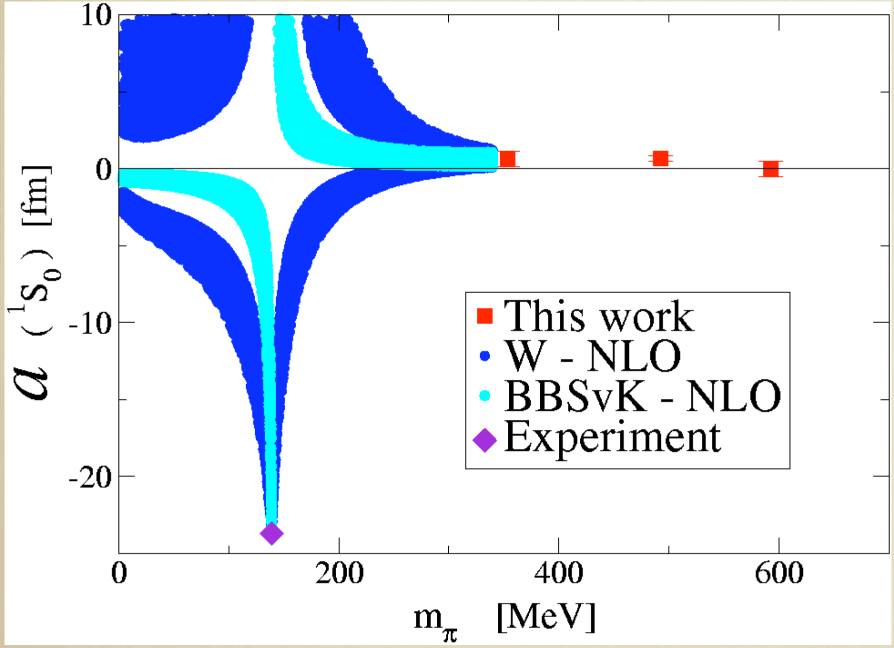


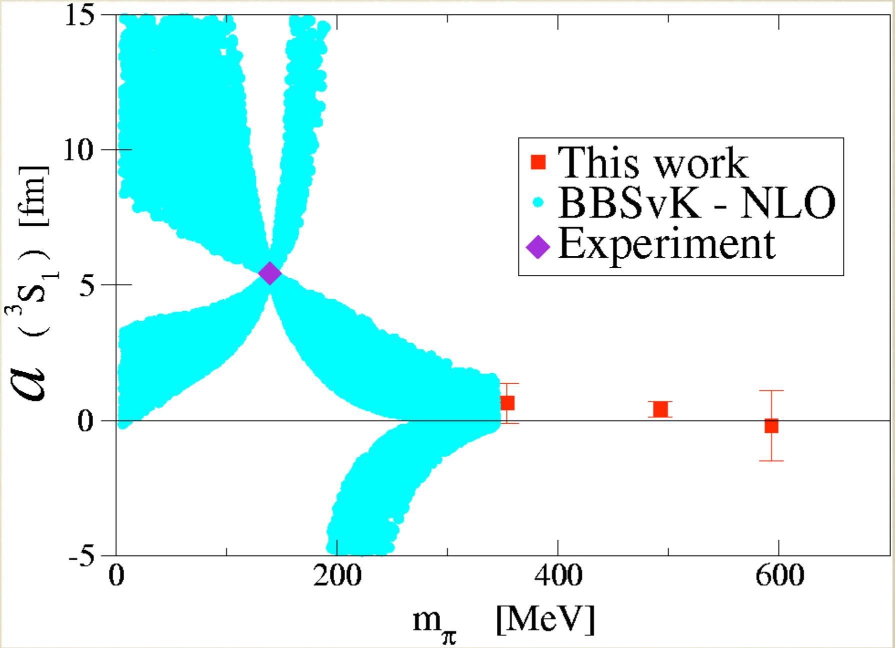
NPLQCD hep-lat/0506013

Nucleon-nucleon scattering length

Large N-N scattering length much more demanding

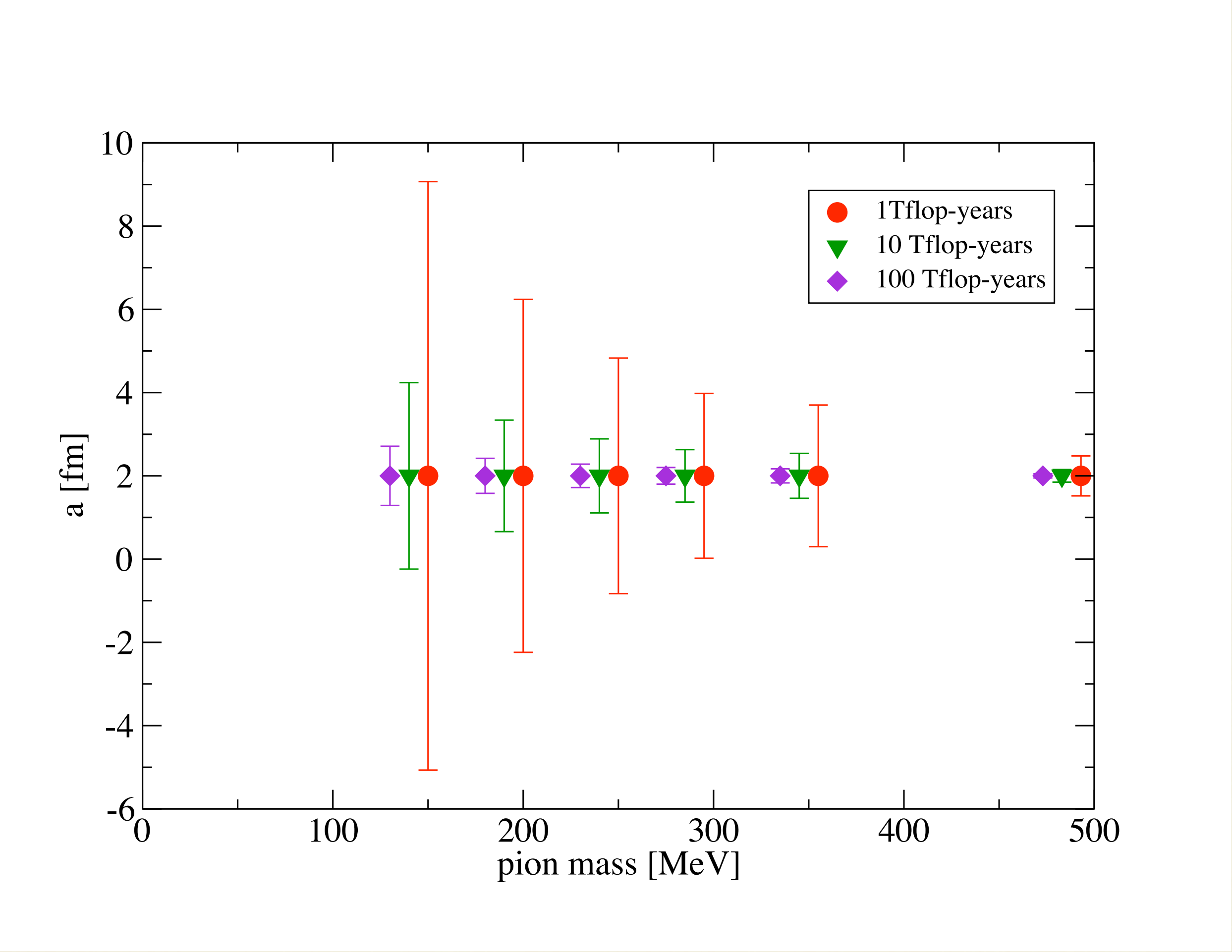
Requires calculation far closer to chiral limit





NPLQCD hep-lat/0602010

Nucleon interactions: projected errors

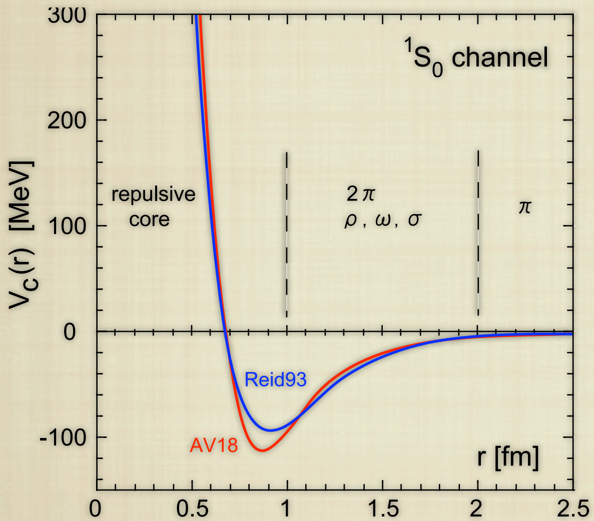


Errors on nucleon-nucleon scattering length as a function of computational resources [NPLQCD]

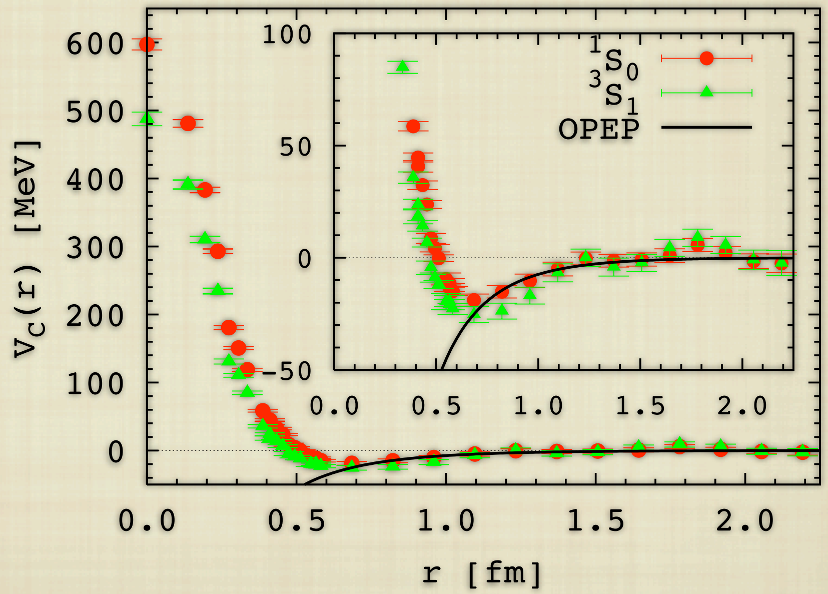
Nucleon-nucleon potential

Nucleon-nucleon potential defined from Bethe-Salpeter wave function calculated in quenched lattice QCD

Ishii, Aoki, Hatsuda, nucl-th/0611096



phenomenology



quenched lattice QCD

Future Prospects

What can one imagine doing in lattice QCD with Petaflops? With Exaflops?

- Precision understanding of quark and gluon structure of nucleons
  - Spectrum of low-lying mesons and baryons, including exotics, and their production form factors
- Equation of state of matter at finite baryon density?
  - Understand QCD phase diagram and neutron stars
- Quantitative understanding of n-n interactions?
- Light nuclei??
  - Combine effective field theory and lattice calculations
- Fundamental input to heavy nuclei???
  - Use parameters of effective field theory in ab initio nuclear many-body calculations

Capability Hardware

- QCD has always driven the development of capability hardware
- QCD Teraflops Project 1992
  - MIT LCS, Physics, Lincoln, TMC, 40 QCD physicists
- QCDSP 1993-1998 Columbia University
  - 0.6Tf peak, 0.18 sustained, $10/sustained Mf, Bell Prize
  - DSP based, low power, mesh communications
  - After completion, Alan Gara joined IBM Watson
- QCDOC (QCD On a Chip)
  - Columbia, RIKEN BNL, Edinburgh, IBM
  - 10Tf peak, ~4Tf sustained, ~$1/sustained Mf
  - Processor, memory, comm. controller on chip

Capability Hardware

- Blue Gene/L
  - Al Gara recognized commercial potential, recruited Dong Chen, James Sexton, Pavlos Vranas
  - QCDOC concept, added:
    tree network
    2 proc/node, 2 fpu/proc.
- QCD physicists interacting strongly with IBM on BG/Q
- Studying future options with O(100) cores/chip

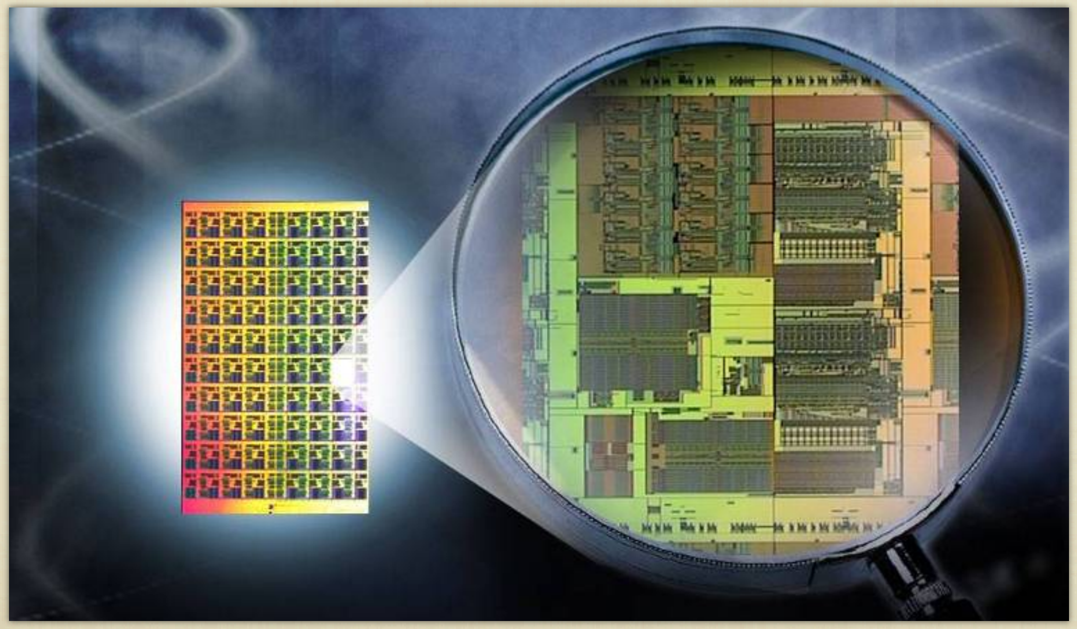
Optimized platform-independent software

- Layered SciDAC API
  - High level platform independent physics code
  - Low level routines optimized to each platform
- Metaprograming -
  facilitate optimization on evolving architectures
  - QDP
  - Vector abstraction
  - Q language
  - Cache oblivious algorithms
- Both highly relevant to ASC

Multicore

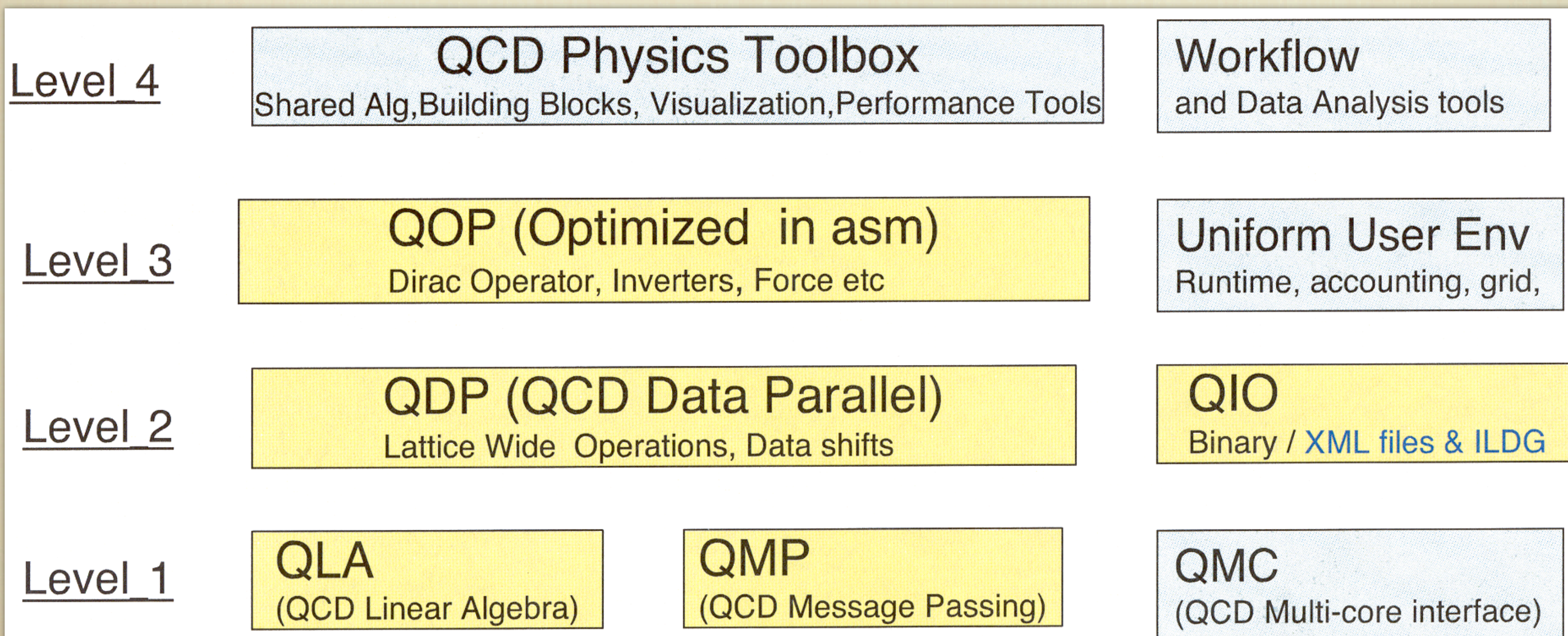
- Essential to design software with appropriate structure and abstractions to better exploit emerging multicore architectures

- Example: Intel's 2-11-07 announcement of 80 core chip achieving 1.01 Tflps at 3.16 Ghz with 62 watts



SciDAC API

- 5 year SciDAC software effort - continue in SciDAC-2
  - Avoid duplication of effort, rewriting for new systems
  - Massive resource needs motivates high efficiency
- Runs on
  - Intel, AMD, Power PC processors
  - BG, Cray XT3, clusters, QCDOC

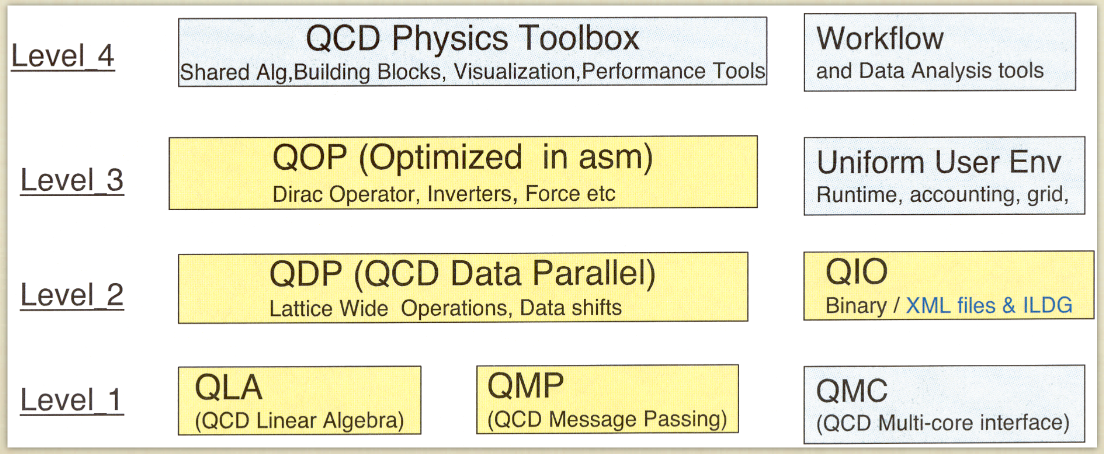


Metaprogramming

- Facilitate optimization on evolving sequence of architectures - moving target
  - Expressive power
  - Appropriate abstractions
  - Optimization tools
- Example: QDP QCD Data Parallel layer

QDP - data parallel layer

- Viewed from above, see parallel data flow
- QMP simpler than MPI
- Hence, we can implement it more efficiently



Vector abstraction

- Back to the future with vector features
  - SSE extended instructions (graphics) X86 Intel and AMD
  - Altivec Power PC
  - BG/L Double Hummer

ops/clock	SSE	Altivec	Double Hummer	QCDOC
SP	4	4	2	
DP	2		2	
no vector	1	1	1	1

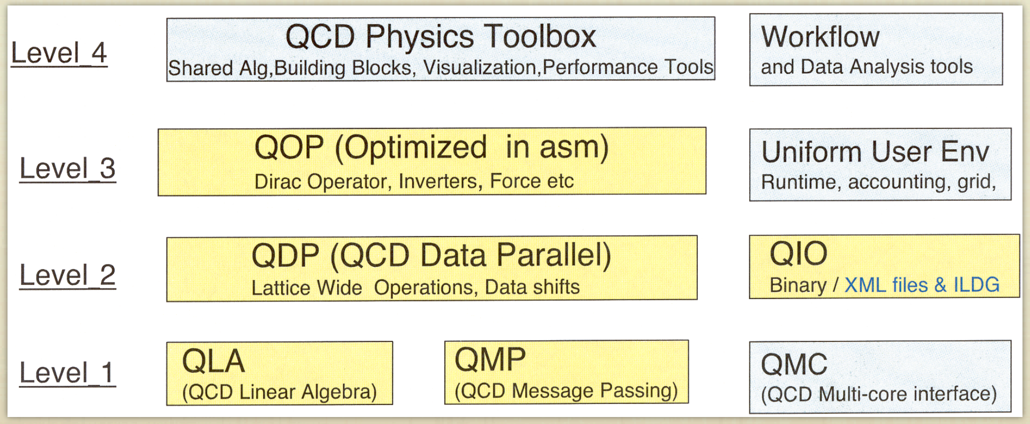
Vector abstraction

- Pochinsky ported gcc compiler producing optimized vector code on BG/L double hummer and <u>all</u> <u>other</u> Scidac platforms
- Algorithmic observation for Conjugate Gradient
  - On SSE and Altivec, first solve in SP, correct in DP
  - Example ~2000 iter SP + ~20 iter DP
  - Built into SciDAC software - DP at half the cost or less on some platforms.
- Still need to implement BG complex (a * b+c)

ops/clock	SSE	Altivec	Double Hummer	QCDOC
SP	4	4	2	
DP	2		2	
no vector	1	1	1	1

Q language

- Pochinsky wrote Q to integrate QDP into its language features
- Used to generate some QLA routines.
- In future, generalize as tool for optimized low level routines on BG/P, BG/Q

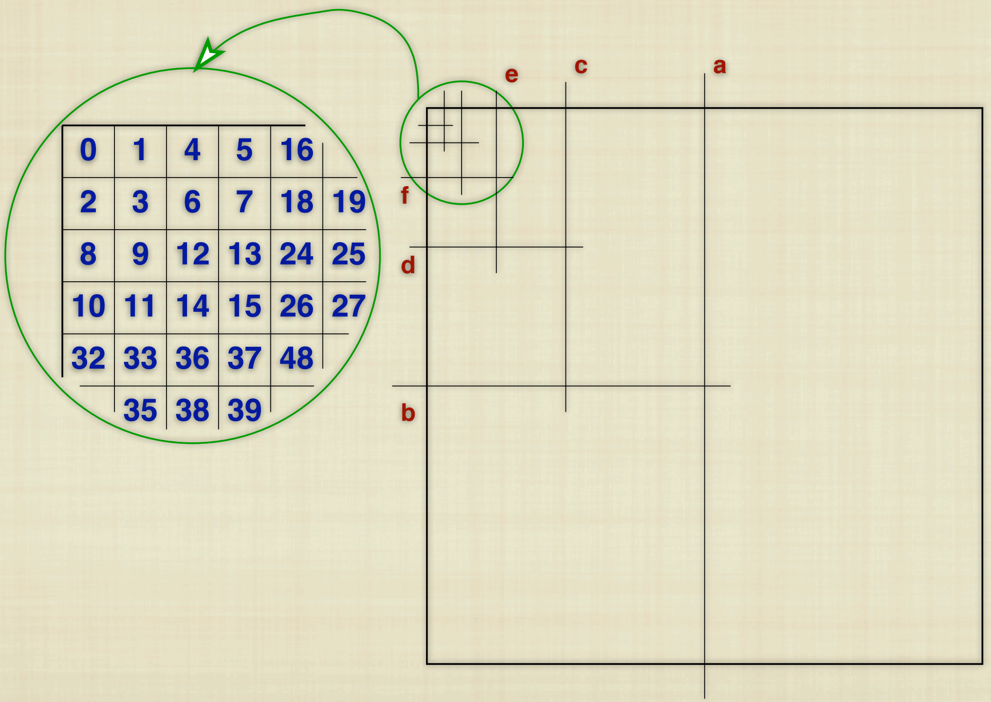


Cache oblivious algorithms

- Memory bandwidth is crucial limitation
  - Most chips designed for sweet spot in marketplace, not cycle-mongers like us
  - QCDOC → BG/L
    4 x processing power, but not 4 x bandwidth
  - Algorithms already organized for maximum reuse
- Efficient utilization of (small) on-chip cache essential
  - Meticulous hand coding excruciating
  - Observe huge layout dependence without it

Cache oblivious algorithms

- Pochinsky is organizing layout to be optimal for any cache



MIT Blue Gene Project

- Working with SciDAC collaborators, Pochinsky and Khoriaty have ported all relevant SciDAC software to BG/L
- Pochinsky is developing tools, including gcc compiler and Q, for porting to BG/P and Q
- Pochinsky has written optimized Level 3 inverter for BG/L
- Jahn is developing an optimized eigenvalue solver for BG/L
- Pochinsky and JN are completing an intellectual property agreement between MIT and IBM providing access to proprietary information required for further optimization

Ambitions for the Future

- Solve increasingly difficult fundamental QCD problems
  - Nucleons and equation of state at zero density
  - Nuclear interactions and e.o.s. at non-zero density
  - Potential for fundamental input to calculations of nuclei
- Continue to push the envelope on capacity architectures
  - Interact strongly with IBM on BG/Q
  - Explore future options with O(100) cores/chip
- Implement vision of platform independent optimized software
  - Complete the SciDAC API
  - Develop metaprogramming and automated optimization tools
  - Transfer as much as possible to ASC community
- Attract gifted graduate students into computational science